dr. V. Šips

Uvod u atomsku mehaniku II

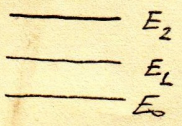
(1 - 30)

Zračenje crnog tijela

$$U_\omega = \frac{dU}{d\omega} = \frac{\omega^2 \bar{E}}{\pi^2 c^3} \qquad \bar{E} = kT$$

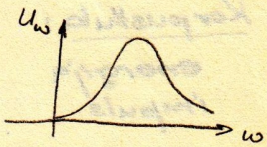
ω, $\omega + d\omega$ Jeans-Rayleigh

- M. Planck

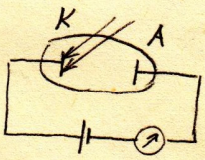


$$E_n = n\hbar\omega \qquad n = 0, 1, 2, \ldots$$

$$\Rightarrow \bar{E} = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$$



- Fotoefekt otkriva Hertz 1888.



- Zakone daje Lenard 1889.

1) $\frac{mV_M^2}{2} = \hbar\omega - J$ — ovisna samo o materiji

2) Energija izlaž. elektrona ne ovisi o intenzitetu

- objašnjava Einstein 1905.

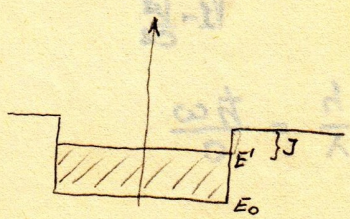
svjetlost od fotona $E = \hbar\omega$

- povezano s kvantiz. harm. oscilatora $\nearrow$ emisija, $\searrow$ anihilacija

$$\hbar\omega = J + \frac{mV_M^2}{2}$$

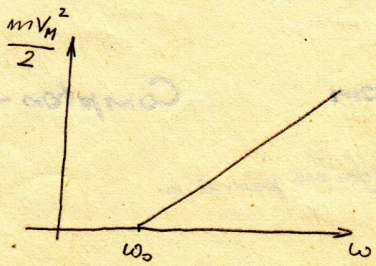
$$eV_i - (eV_a + E_s) + \hbar\omega = \frac{mV_M^2}{2}$$

nella razpodjela kin. energ. u metalu — površ. pot. barijera — gubitak energ. elast. sudarima do površine



$\rightarrow \exists$ minimalna energija

prag fotoefekta $J = \hbar\omega_0$



→ i foton ima impuls

formalno (nekorektan dokaz) jer masa mir. = 0

$E = mc^2$

$p = mc = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda}$

$E = c\sqrt{p^2 + m_0^2 c^2}$

ili quasi čestice: $m_0 = 0$

$h\nu = c \cdot p \Rightarrow p = \frac{h\nu}{c}$

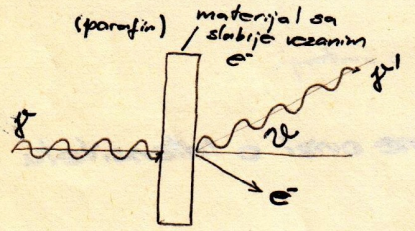
$\vec{p} = \hbar \vec{k}$ $\quad |\vec{k}| = \frac{2\pi}{\lambda}$

Korpuskula:
energija
impuls

$E = h\nu$
$p = \frac{h}{\lambda}$
veza preko h

val:
frekvencija
valna dužina

Compton-ov efekt (1922.)



- izlazni foton je to manje energije, što je jače otklonjen
- pretp. da je e^- mirovao

zakoni konzervacije E & p

$\vec{p} = \vec{p}' + \frac{m\vec{v}}{\sqrt{1-\frac{v^2}{c^2}}}$ $\qquad \hbar\omega + m_0c^2 = \hbar\omega' + \frac{m_0c^2}{\sqrt{1-(\frac{v}{c})^2}}$

$c = \lambda\nu = \lambda \cdot \frac{\omega}{2\pi}$

$\frac{\frac{h}{2\pi}}{\frac{\lambda}{2\pi}} = \frac{\hbar}{\frac{c}{\omega}}$

$p = \frac{h}{\lambda} = \frac{\hbar\omega}{c}$ $\qquad p' = \frac{\hbar\omega'}{c}$

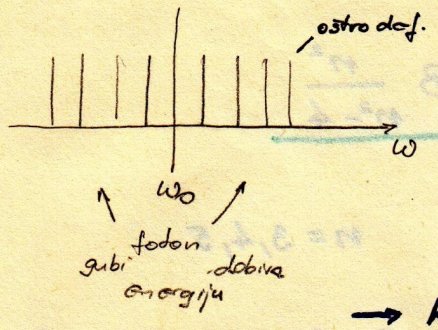
$\Rightarrow \Delta\lambda = \lambda' - \lambda = 2\lambda_c \sin^2\frac{\vartheta}{2}$

$\lambda_c = \frac{h}{mc} = 2{,}42 \cdot 10^{-8}\,cm$ $\qquad$ Compton-ova valna dužina

$\approx 10^{-8}\,cm$

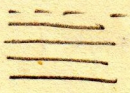
rentgensko područje

Ramanov efekt (1928)



- monokrom. el.m. val pada na tek ili plinove izlazni el.m. val tada se pojavljuje i sa drugim frekvencijama koje su više ili niže od poč. frekvencije
(dok kod Compt. su uvijek niže frekv.)

→ Kvantizirane energije molekula
doznajemo kvantna stanja molekule
(preslikavamo rezultat u energ. nivoe molek.)



Spektralna analiza: (Bunsen, Kirchof, ...)

plinovi - linije apsorbcije i emisije leže na istom mjestu
otkrivanje novih elemenata Rb, Cs, He

1A plinovi - atomi dovoljno daleko → nema interakcije - svodise na proučavanje (jednake) atoma
tj. N nezav. sistema

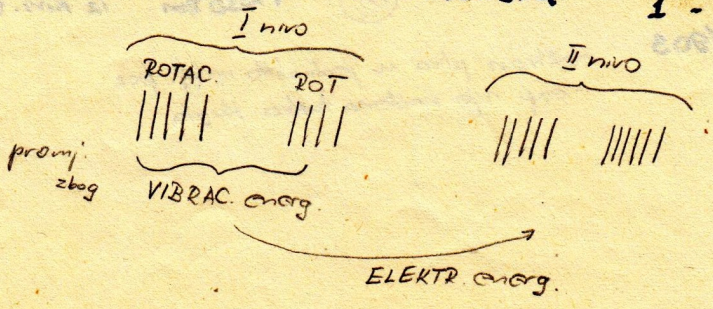
→ **Atomski spektar:**
linije

H : $\lambda_\alpha = 6563$ Å
$\lambda_\beta = 4869$ Å
$\lambda_\gamma = 4341$ Å
$\lambda_\delta = 4102$ Å
⋮

elektronska energija → linijski spektar

→ **Molekule:** energije - Rotaciona $10^{-5} - 10^{-3}$ eV
Vibraciona $10^{-2} - 10^{-1}$ eV
Elektronska $1 - 10$ eV najveća

} vrpčasti spektar



Balmer (1885)

1° nagomilavanje linija (linijski spektri)

2° empirijska formula $\lambda = B \frac{n^2}{n^2-4}$

$$\frac{1}{\lambda} = \overset{R}{\frac{1}{B}}\left(1-\frac{4}{n^2}\right) = \frac{4}{B}\left(\frac{1}{2^2}-\frac{1}{n^2}\right) \qquad n = 3,4,5\ldots$$

$$\nu = \frac{c}{\lambda} = c\underset{Z^2}{R}\left(\frac{1}{2^2}-\frac{1}{n^2}\right) \qquad \text{Rydberg} \quad R = 109677{,}58\ \mathrm{cm}^{-1}$$

Kasnije:

Lyman-ova serija

$$\nu = cR\left(\frac{1}{1^2}-\frac{1}{n^2}\right) \qquad n = 2,3,4,\ldots$$

Paschen ... $\frac{1}{3^2}$ .. $n = 4,5,\ldots$

Bracket ... $\frac{1}{4^2}$ .. $n = 5,6,\ldots$

Pfund ... $\frac{1}{5^2}$ .. $n = 6,7,\ldots$

3° Rydberg, Ritz

princip kombinacija terma T_1, T_2, T_3, T_4

$$\omega_{nn'} = T_n - T_{n'} \qquad T_n = -\frac{E_n}{hc}$$

$$h\nu_{nn'} = E_n - E_{n'} > 0$$

$$\nu_{nn'} = \frac{E_n}{h} - \frac{E_{n'}}{h}$$

$$\omega_{nn'} = (T_n - T_\ell) + (T_\ell - T_{n'}) = \omega_{n\ell} + \omega_{\ell n'}$$

4° Pokušaj mikroskopskog objašnjenja

- uloga atomskog modela: (+) $r \approx 10^{-8}$ cm iz kin. teorije

Thomson 1903

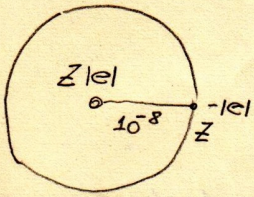
elektron pliva u jednolito nabij. poz

- exp. nije nađena takva kugla

→ Rutherford (1911 - 1913)

raspršenje α-zraka → samo mali dio zraka doživljava otklon

→ planetarni model

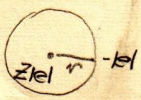


1 fermi

$1 f = 10^{-13}$ cm

uspješnost - klas. teorije

- Maxwell : titranje dipola → el.m. zračenje frekvencije titranja dipola



energija za gib. po kružnici. - zračenjem se smanjuje

$E = -\frac{Ze^2}{2a}$ $a = r$ postaje sve negativnija → a se smanjuje

→ gibanje po spirali → mijenjanje ν - suprotno exp.

$\approx 10^{-8}$ s pad na jezgru

- gibanje po elipsi još teže -

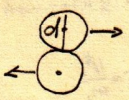
neharmonijsko gibanje → Fourier. red.

$$x(t) = \sum_{k=0}^{\infty} a_k e^{ik\omega t}$$

$\omega, 2\omega, \dots, k\omega, \dots$ frekvencije

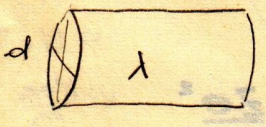
ne opažaju se

- atomi u plinu se sudaraju bezbroj x



πd^2 udarni presjek

N atom/cm³



$\lambda \pi d^2 \cdot N = 1$ atom

put, pa da atom naiđe na drugi

$\lambda = \frac{1}{\pi d^2 N}$ $N \approx 10^{20}/cm^3$ $d \approx 10^{-8}$ cm ⇒ $\lambda \approx 10^{-4}$ cm

sr. slob. put

relaksacijno vrijeme (između dva sudara)

$\lambda = v \cdot \tau$

$v \approx \sqrt{\frac{kT}{M}} \approx 10^5$ cm/s ⇒ $\tau \approx 10^{-9}$ s mnogo sudara u 1s →

→ perturbacije, a emitirani spektar je postojan!

dok u sunčevu sistemu izvjesno uzrok velik perturbacija

- niz teškoća u mikroskopskom području

N. Bohr-ovi postulati (1913)

„pogreška je bila u klas. interpret. zračenja"

1) boravak el. u stac. stanjima (energetskim)

$$E_0, E_1, E_2, \dots$$

Atom ostaje u osnovnom stac. stanju sve dok ne dobije dovoljno energije za prijelaz u više

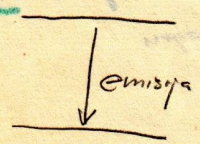
2) el. u jednom stac. stanju ne emitira el. m. val

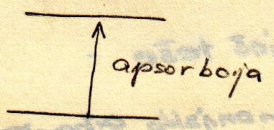
do emisije dolazi tek kad elektron prelazi iz višeg energ. stanja u niže

$$\omega_{nn'} = \frac{E_n - E_{n'}}{\hbar}$$

$$\omega_{nn'} = \frac{E_n - E_l}{\hbar} + \frac{E_l - E_{n'}}{\hbar} = \omega_{nl} + \omega_{ln'}$$

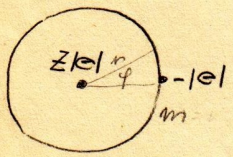
dobili smo i kombinacioni princip





- bijela svjetlost → apsorbcija nekih spektr. linija

→ Račun energ. stac. stanja & ω



$Z = 1$ H

$Z = 2$ He^+

$Z = 3$ Li^{++}

$p_i = \frac{\partial L}{\partial \dot{q}_i}$

$H = E_k + U$ za Konz sile & Klas. meh.

$\dot{q}_i = \frac{\partial H}{\partial p_i}$ $\dot{p}_i = -\frac{\partial H}{\partial q_i}$

$$E_k = \frac{m}{2}(\overset{v^2}{\dot{r}^2 + r^2\dot{\varphi}^2})$$

$$p_\varphi = \frac{\partial E_k}{\partial \dot{\varphi}} = mr^2\dot{\varphi}$$

$C = \frac{|\vec{r}|}{m_2}$

$$\vec{F}_{12} = \frac{Km_2}{r^2}\vec{r}_{01}$$

$-\frac{\partial U}{\partial r}$

$\Rightarrow U = \frac{Km_2}{r^2}$

$$a_r = \ddot{r} - r\dot{\varphi}^2$$

$$a_\varphi = \frac{1}{r}\frac{d}{dt}(r^2\dot{\varphi})$$

$$\dot{p}_\varphi = -\frac{\partial H}{\partial \varphi} \qquad U = -\frac{Ze^2}{r}$$

$K = \frac{k^2 e_1 e_2}{m_2}$ $k^2 = 1$ cgs.

$e_1 = +Z|e|$

$e_2 = -|e|$

$= 0 + 0$

$\Rightarrow p_\varphi = const.$ II Kepler. zakon

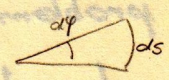
gdje sila centralna ⇒ gibanje u jednoj ravni.

→ Konstanta gibanja koju će Bohr kvantizirati.

$$p_\varphi = mr^2\dot{\varphi} = m\cdot\frac{|\vec{r}|}{m} = |\vec{r}| = |\vec{R}\times m\vec{v}|$$

$$r\vec{r}_0 \times m(\dot{r}\vec{r}_0 + r\dot{\varphi}\vec{\varphi}_0) = r^2\dot{\varphi}\ \vec{r}_0\times\vec{\varphi}_0$$

Kružica: $\dot{r}=0$ $\quad v = r\dot{\varphi}$ $\quad a_r = -\frac{v^2}{r} = -r\dot{\varphi}^2$ $\quad a_\varphi = r\ddot{\varphi}$



$ds = r\,d\varphi \Rightarrow v = r\dot{\varphi}$

$v = \sqrt{\frac{|K|}{r}}$ $\quad K = \frac{1\cdot e_1 e_2}{m_2}$

$$\frac{mv^2}{r} = +\frac{Ze^2}{r^2} \quad /\cdot r^2$$

$$p_\varphi = \underbrace{mrv}_{|\vec{p}|} = M = |\vec{p}|$$ angularni moment (moment impulsa) : solenoid

$$mrv^2 = +Ze^2$$

$$\Rightarrow v = \frac{Ze^2}{p_\varphi}$$

$$E = \frac{mv^2}{2} - \frac{Ze^2}{r} = -\frac{Ze^2}{2r} = -\frac{m_2 K^2}{2C^2}$$

$E<0$

$K = \frac{1\cdot Ze(-e)}{m_2}$

$C = \frac{\Gamma}{m} = |\vec{r}\times\vec{v}| = r\cdot v$

$$= -\frac{mZe^2\cdot Ze^2}{2\cdot r^2 v^2\cdot m^2} = -\frac{mZe^2}{2r}\cdot\frac{Ze^2}{mrv^2} = 1$$

$$r = \frac{p_\varphi}{mv} = \frac{p_\varphi^2}{mZe^2}$$

$$E = -\frac{(k)^2 mZ^2e^4}{2p_\varphi^2}$$ $k^2=1$ (cgs sustav)

$$p_\varphi = n\hbar$$

→ Bohr kvantizira konst. gibanja p_φ, da bi kvantizirao E

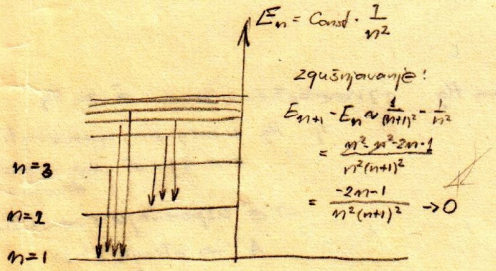
$$v_n = \frac{Ze^2}{n\hbar} \qquad r_n = \frac{n^2\hbar^2}{mZe^2} \qquad E_n = -\frac{mZ^2e^4}{2n^2\hbar^2} \qquad \omega_n = \frac{v}{r} = \frac{mZ^2e^4}{n^3\hbar^3}$$

$n=1$ ≡ 0 nivo

$Z=1$

$$v_0 = \frac{e^2}{\hbar} = 2{,}2\cdot 10^8\ \frac{cm}{s} \qquad E_0 = -\frac{me^4}{2\hbar^2} = -2{,}18\cdot 10^{-11}\ erg$$

$$r_0 = \frac{\hbar^2}{me^2} = 0{,}529\cdot 10^{-8}\ cm$$



$$\omega_{nn'} = \frac{E_n - E_{n'}}{\hbar} = \frac{mZ^2e^4}{2\hbar^3}\left(\frac{1}{n'^2}-\frac{1}{n^2}\right)$$

$$\nu_{nn'} = \frac{1}{2\pi}\omega_{nn'} = C\,Z^2\underbrace{\frac{me^4}{4\pi c\hbar^3}}_{R_0}\left(\frac{1}{n'^2}-\frac{1}{n^2}\right)$$

izraō: Rydberg. konst. $R_0 = 109\,737{,}3\ cm^{-1}$

exp. za H $\quad R = 109\,677{,}6\ cm^{-1}$

} gotovo max slaganje

$\ddot{\vec{r}} = \frac{K}{r^2}\vec{r}_0$

$\mu\ddot{\vec{r}} = \vec{F}_{12} = \frac{Km_2}{r^2}\vec{r}_{01} \Rightarrow \ddot{\vec{r}} = \frac{\overbrace{Km_2}^{K'}}{\mu r^2}\vec{r}_{01}$ $\quad = (\vec{r}\times\vec{v})$ $\quad C = \frac{\Gamma}{m_2}$

$E = \frac{1}{2}\mu\dot{\vec{r}}^2 + \frac{Km_2}{r}$ $\quad r = \frac{p}{-1\pm\varepsilon\cos\varphi}$ $\quad p = \frac{C^2}{|K'|}$

$\varepsilon = \sqrt{1+\frac{2EC^2}{\mu K'^2}}$

→ **problem dva tijela - bolje slaganje**

$$\frac{1}{\mu} = \frac{1}{\underset{m_1}{m}} + \frac{1}{\underset{m_2}{M}}$$

Kružica! $\varepsilon = 0 \Rightarrow E = -\frac{\mu K'^2}{2C^2}$ $\quad (*)$ $\quad r = p = \frac{C^2}{|K'|}$ $\quad \dot{r} = 0 \Rightarrow v = r\dot{\varphi}$

$\frac{m_2}{\mu}\cdot n\hbar = \text{const.} = {}_{\shortparallel}p_\varphi{}_{\shortparallel} = m_2 \overset{C}{r^2\dot{\varphi}} = m_2 r V \Rightarrow r = \frac{{}_{\shortparallel}p_\varphi{}_{\shortparallel}}{m_2 V}$ $\quad (*) \Rightarrow V = \sqrt{\frac{|K'|}{r}}$ $\quad v^2 = \frac{K'^2}{C^2} - \frac{2K'}{r} = \frac{K'}{r} - \frac{2\varepsilon K'}{r}$

$|K'| = \frac{m_2}{\mu}\frac{k^2Ze^2}{m_2}$

originalno: & Supek (386)

ovdje moramo kvantizirati ukupan impuls

$n\hbar = |\vec{J}'| = |\vec{r}_1'\times m_1\dot{\vec{r}}_1' + \vec{r}_2'\times m_2\dot{\vec{r}}_2'| = |\vec{r}\times\mu\dot{\vec{r}}| = |\vec{C}'| = \mu r^2\dot{\varphi}$

$\Rightarrow m_2 r V^2 = \frac{m_2}{\mu}\overset{k^2}{\underset{1}{}}Ze^2 \Rightarrow V = \frac{\frac{m_2}{\mu}Ze^2}{{}_{\shortparallel}p_\varphi{}_{\shortparallel}}$ $\quad r = \frac{{}_{\shortparallel}p_\varphi^2{}_{\shortparallel}}{\frac{m_2}{\mu}Ze^2\cdot m_2}$

$E = \frac{Ze^2}{2r} - \frac{Ze^2}{r} = -\frac{Ze^2}{2r} = -\frac{\frac{m_2}{\mu}Z^2e^4m_2}{2\,{}_{\shortparallel}p_\varphi^2{}_{\shortparallel}}$ $\quad E = -\frac{\frac{m_2}{\mu}Z^2e^4m_2}{2\,{}_{\shortparallel}p_\varphi^2{}_{\shortparallel}}$

$\Rightarrow n\hbar = \frac{\mu}{m_2}\cdot{}_{\shortparallel}p_\varphi{}_{\shortparallel} \Rightarrow {}_{\shortparallel}p_\varphi{}_{\shortparallel} = \frac{m_2}{\mu}\cdot n\hbar$

$$E_n = -\frac{\left(\frac{m}{\mu}\right)^{-1}\cdot mZ^2e^4}{2\hbar^2n^2}$$

$\frac{m_2}{\mu}$ $\quad \left(\frac{m_2}{\mu}\right)^2$

(*) ${}_{\shortparallel}p_\varphi{}_{\shortparallel} = m_2 C$ jer $p_\varphi = \frac{\partial}{\partial\dot{\varphi}}\left[\frac{\mu}{2}(\dot{r}^2+r^2\dot{\varphi}^2) - \frac{Ze^2}{r}\right] = \mu r^2\dot{\varphi}$

$\frac{1}{2\pi}\frac{E_n - E_{n'}}{\hbar}$

$$\nu_{nn'} = CZ^2\cdot\left(\frac{m}{\mu}\right)^{-1}\cdot\underbrace{\frac{me^4}{4\pi\hbar^3C}}_{R_0}\left(\frac{1}{n'^2}-\frac{1}{n^2}\right)$$

$R = \left(\frac{m}{\mu}\right)^{-1}R_0 = \left(\frac{m}{\frac{mM}{m+M}}\right)^{-1}R_0 = \frac{M}{m+M}R_0$

$$\Rightarrow R = \frac{1}{\left(1+\frac{m}{M}\right)}R_0$$

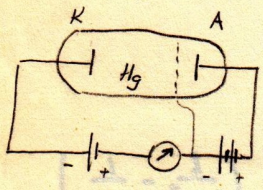
za normalni vodik M

$$R_D = \frac{R_0}{1+\frac{m}{2M}}$$

za teški vodik - deuterij $2M$ (proton + neutron)

→ ustanovimo količ. jednog izotopa u smjesi iz omjera intenziteta pripadnih linija H & D

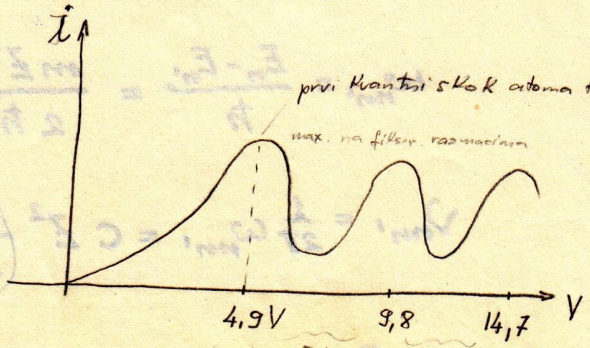
Franck - Hertz



- neg. mrežica štiti A

- mjerili el. struju u balonu s Hg (para) - sudari e^- sa Hg

ionizacioni potencijal (napon) kad poteče struja



→ neelastičan sraz e^- sa Hg

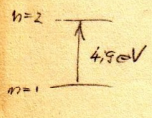
tj. Hg u mogućn. apsorbirati energiju e^-, koja je postala dovoljno velika

⇒ e^- usporavaju i ne stižu na A → struja slabi

za malu energiju e^-

→ **sudari elastični**

dok ćak kasnije dva puta izgubi isto pa sve manji broj e^- može doći na A



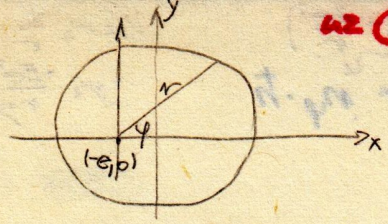
$$\frac{mV^2}{2} = eV$$

→ pobuđeni Hg emitiraju svjetlost

→ exp. dokazan 2) Bohr-ov postulat

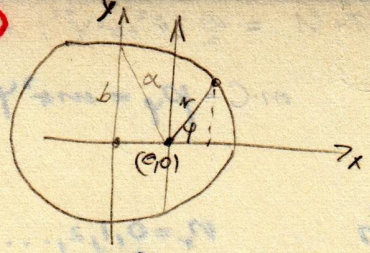
→ prvi rezonantni udarac nastupa kod 4,9 V → $\lambda = 2537$ Å

$\Rightarrow eV = h\nu = h\cdot\frac{c}{\lambda}$



$-\varepsilon$

$0<\varepsilon<1$



$+\varepsilon$

$$r=\frac{p}{1\mp\varepsilon\cos\varphi}$$

$$\varepsilon=\frac{e}{a}$$

$$b^2=a^2-e^2$$

$$r=\sqrt{(x\pm e)^2+y^2} \qquad \cos\varphi=\frac{x\pm e}{r}$$

$$p=\frac{b^2}{a}$$

$$r\mp\varepsilon\cdot\cancel{r}\cdot\frac{(x\pm e)}{\cancel{r}}=p$$

$$r\mp\varepsilon x\mp e\cdot\varepsilon=p$$

$$r=(p\mp e\cdot\varepsilon)\pm\varepsilon x \quad /^2$$

$$(x\pm e)^2+y^2=(p\mp e\varepsilon)^2\pm 2\varepsilon(p\mp e\varepsilon)x+\varepsilon^2x^2$$

$$x^2\pm 2ex+e^2+y^2=p^2\mp 2e\varepsilon p+e^2\varepsilon^2\pm 2\varepsilon px\pm 2e\varepsilon^2x+\varepsilon^2x^2$$

$$\underbrace{(1-\varepsilon^2)}_{\frac{b^2}{a^2}}x^2+x(\pm 2e\mp 2\varepsilon p\mp 2e\varepsilon^2)+y^2=p^2\mp 2e\varepsilon p+e^2\varepsilon^2-e^2$$

zahtjev: neporemaćena elipsa

$$\pm 2e\mp 2\varepsilon p\mp 2e\varepsilon^2=0$$

$$e-\varepsilon p-e\varepsilon^2=0 \Rightarrow p=\frac{e(1-\varepsilon^2)}{+\varepsilon}=\frac{e\cdot\frac{b^2}{a^2}}{\frac{e}{a}}$$

$$\Rightarrow \boxed{p=\frac{b^2}{a}}$$

$$\frac{\partial L}{\partial \dot r} \qquad L = T - U = \frac{m}{2}(\dot r^2 + r^2\dot\varphi^2) - \underbrace{\left(-\frac{Ze^2}{r}\right)}_{U} \qquad U = m_2\frac{K}{r} = \frac{ZE(-E)}{m_2}$$

$$= \cancel{m_2}\cdot\frac{-Ze^2}{r\,\cancel{m_2}}$$

$$p_r = \frac{\partial E_u}{\partial \dot r} = m\dot r \qquad m\cdot C = p_\varphi = mr^2\dot\varphi = n_\varphi\cdot\hbar$$

$$\oint p_r\,dr = n_r\cdot h \qquad n_r = 0,1,2,\dots$$

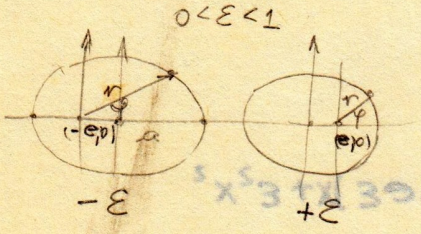
$$r = \frac{p\,\mathrm{sg}K}{-1 \pm \varepsilon\cos\varphi} \qquad \mathrm{sg}K = -1 \qquad K = -\frac{Ze^2}{m_2}$$

$$p = \frac{C^2}{|K|} = \frac{p_\varphi^2}{mZe^2}$$

$$r = \frac{\frac{p_\varphi^2}{mZe^2}}{1 \mp \varepsilon\cos\varphi} \qquad p$$

$$dr = \frac{p}{(1 \mp \varepsilon\cos\varphi)^2}(\pm\varepsilon\sin\varphi)\,d\varphi$$

$0 < \varepsilon < 1$



$$\dot r = \frac{p}{(1 \mp \varepsilon\cos\varphi)^2}(\pm\varepsilon\sin\varphi)\cdot\dot\varphi$$

$$= \frac{p}{(1 \mp \varepsilon\cos\varphi)^2}(\pm\varepsilon\sin\varphi)\cdot\frac{p_\varphi}{m}\cdot\frac{1}{r^2}$$

$$\Rightarrow \dot r = \frac{p}{\cancel{(1 \mp \varepsilon\cos\varphi)^2}}(\pm\varepsilon\sin\varphi)\cdot\frac{p_\varphi}{m}\cdot\frac{\cancel{(1 \mp \varepsilon\cos\varphi)^2}}{p^2}$$

$$\dot r = \frac{p_\varphi}{m\cdot p}(\pm\varepsilon\sin\varphi)$$

$$\Rightarrow p_r = \frac{p_\varphi}{p}(\pm\varepsilon\sin\varphi)$$

$$p_r = \frac{mZe^2}{p_\varphi}(\pm\varepsilon\sin\varphi)$$

*) str 5

$$E = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\varphi}^2\right) - \frac{Ze^2}{r} \qquad C = r^2\dot{\varphi} \qquad k = \frac{k^2 e_1 e_2}{m_2} = -\frac{Ze^2}{m}$$

$$E = \frac{m}{2}\left(\dot{r}^2 + \frac{C^2}{r^2}\right) - \frac{Ze^2}{r} \qquad p = \frac{C^2}{|k|} = \frac{mC^2}{Ze^2}$$

za $\dot{r} = 0$ $\quad r = r_{extr.} = r_{min,max}$

$$E = \frac{m}{2}\cdot\frac{C^2}{r_{extr.}^2} - \frac{Ze^2}{r_{extr}} \qquad r_{extr.} = \frac{p}{1 \mp \varepsilon}$$

$$E = \frac{mC^2}{2p^2}\cdot(1 \mp \varepsilon)^2 - \frac{Ze^2}{p}(1 \mp \varepsilon)$$

$$E = \frac{mC^2}{2p^2} \mp \cancel{\frac{mC^2}{p^2}\varepsilon} + \frac{mC^2}{2p^2}\varepsilon^2 - \frac{Ze^2}{p} \pm \cancel{\frac{Ze^2}{p}\varepsilon}$$

$$E = \frac{mC^2}{2p^2}(1+\varepsilon^2) - \frac{Ze^2}{p} \qquad Ze^2 p \qquad \frac{Ze^2}{p} = \frac{Ze^2 p}{p^2} = \frac{mC^2}{p^2}$$

$$E = \frac{Ze^2}{2p}(1+\varepsilon^2) - \frac{Ze^2}{p}$$

$$E = -\frac{Ze^2}{2}\left[\frac{2}{p} - \frac{(1+\varepsilon^2)}{p}\right]$$

$$E = -\frac{Ze^2}{2}\cdot\frac{2-1-\varepsilon^2}{p} = \frac{1-\varepsilon^2}{p} = \frac{1-\frac{e^2}{a^2}}{\frac{b^2}{a}} = \frac{a^2-e^2}{ab^2} = \frac{b^2}{ab^2} = \frac{1}{a}$$

$$\boxed{E = -\frac{Ze^2}{2a}}$$

*)' uz (5)

Problem dva tijela - ukupna energija (Konz. sile - centralna & Klas. meh.)

$$E = H = T + U = \frac{1}{2}\mu \dot{\vec{r}}^2 + \frac{K m_2}{r}$$

$$K' = \frac{m_2}{\mu} K = -\frac{Ze^2}{\mu}$$

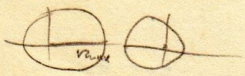
$$K = -\frac{Ze^2}{m_2} \qquad k^2 = 1$$

$$E = \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\varphi}^2) + \frac{K m_2}{r}$$

$p_\varphi = \mu r^2 \dot{\varphi}$ cps.

$$C = \frac{|\vec{r}'|}{\mu} = \frac{p_\varphi}{\mu} = r^2\dot{\varphi}$$

$$E = \frac{\mu}{2}\left(\dot{r}^2 + \frac{C^2}{r^2}\right) + \frac{K m_2}{r}$$



$$r = \frac{p}{1 \pm \varepsilon \cos\varphi} \qquad p = \frac{C^2}{|K'|}$$

$$\varepsilon = \sqrt{1 + \frac{2EC^2}{\mu K'^2}} \quad < 1 \text{ pr. } E<0$$

$$\dot{r} = 0 \Rightarrow r = r_{extr} = \frac{p}{1 \pm \varepsilon}$$

$$E = \frac{\mu}{2} \cdot \frac{C^2}{r_{extr.}^2} - \frac{Ze^2}{r_{extr.}}$$

$$\frac{Ze^2}{p} = \frac{Ze^2 p}{p^2} = \frac{\cancel{Ze^2} \cdot \frac{C^2\mu}{\cancel{Ze^2}}}{p^2} = \frac{\mu C^2}{p^2}$$

$$E = \frac{\mu C^2}{2p^2}(1 \pm \varepsilon)^2 - \frac{Ze^2}{p} \cdot (1 \pm \varepsilon)$$

$$E = \frac{Ze^2}{2p} \pm \cancel{\frac{Ze^2}{2p} \cdot 2\varepsilon} + \frac{Ze^2}{2p} \cdot \varepsilon^2 - \frac{Ze^2}{p} \mp \cancel{\frac{Ze^2}{p}\varepsilon}$$

$$E = \frac{Ze^2}{2p}(1 + \varepsilon^2) - \frac{Ze^2}{p} = -\frac{Ze^2}{2p}(2 - 1 - \varepsilon^2) = -\frac{Ze^2}{2p}(1 - \varepsilon^2)$$

$$E = -\frac{Ze^2}{2}\frac{(1 - \varepsilon^2)}{p} = \frac{1 - \frac{e^2}{a^2}}{\frac{b^2}{a}} = \frac{a^2 - e^2}{a \cdot b^2} = \frac{b^2}{a b^2} = \frac{1}{a}$$

$$\Rightarrow \boxed{E = -\frac{Ze^2}{2a}} = -\frac{\mu Z^2 e^4}{2\hbar^2 n^2} \Rightarrow a = \frac{\hbar^2 n^2}{\mu Z e^2}$$

$$\frac{T^2}{a^3} = \frac{4\pi^2 m}{Ze^2}\left(\frac{M}{m+M}\right)$$

M - masa jądra
m - masa elektronu

$$\mu = \frac{mM}{m+M}$$

$$\frac{T^2}{a^2} = \frac{4\pi^2 m}{Ze^2}\left(\frac{M}{m+M}\right)\cdot\frac{\hbar^2 n^2}{\mu Z e^2}$$

$$a = \frac{\hbar^2 n^2}{\mu Z e^2}$$

$$= \frac{4\pi^2\hbar^2 n^2}{Z^2 e^4}\left(\frac{M}{m+M}\right)$$

$$p_\varphi = n_\varphi \hbar$$

$$\frac{T}{a} = \frac{2\pi\hbar n}{Ze^2}$$

$$\cancel{\frac{b^2\pi^2\cdot 4\mu^2}{n_\varphi^2\hbar^2} = \frac{4\pi^2\hbar^2 n^2}{Z^2 e^4}\left(\frac{M}{m+M}\right)}$$

$$b = \frac{n_\varphi\hbar}{2\mu}\cdot a\,\frac{T}{a^2}$$

$\frac{T}{a}\cdot\frac{1}{a}$

$$b = n_\varphi\cdot a\cdot\frac{\hbar}{2\mu}\cdot\frac{2\pi\hbar n}{Ze^2}\cdot\frac{\mu Z e^2}{\hbar^2 n^2}$$

$$\Rightarrow \quad b = a\,\frac{n_\varphi}{n}$$

**) u2 5

$$\oint p_r dr = n_r h \qquad \oint p_\varphi d\varphi = n_\varphi h$$

Konz. sile & nerelativ. meh.

$$H = T + U \qquad L = T - U$$

problem dva tijela : $T = \frac{\mu}{2}(\dot{r}^2 + r^2\dot{\varphi}^2) \qquad U = -\frac{Ze^2}{r}$

$\mu = \frac{m+M}{m \cdot M}$

$$p_r = \frac{\partial L}{\partial \dot{r}} = \mu \dot{r} \qquad p_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = \mu r^2 \dot{\varphi}$$

$$\dot{p}_\varphi = -\frac{\partial H}{\partial \varphi} = 0 \Rightarrow p_\varphi = \text{const.}$$

$$\Rightarrow p_\varphi = n_\varphi \hbar$$

$$E = H = \frac{1}{2\mu}\left(p_r^2 + \frac{n_\varphi^2 \hbar^2}{r^2}\right) - \frac{Ze^2}{r}$$

$$\Rightarrow p_r = \pm\left(2\mu E + \frac{2\mu Z e^2}{r} - \frac{n_\varphi^2 \hbar^2}{r^2}\right)^{1/2}$$

$$\oint p_r dr = n_r h \Rightarrow \boxed{E = -\frac{\mu Z^2 e^4}{2\hbar^2 (n_r + n_\varphi)^2}}$$

$H = T + U$

$E = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$ $\quad x=0 \quad E = \frac{m^2 v^2}{2m}$

$t=0 \quad x=0 \quad \dot{x} = v$

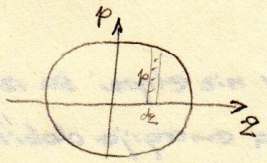
$x = \frac{v}{\omega} \sin\omega t$

$\dot{x} = v \cos\omega t \quad p = m\dot{x} = mv\cos\omega t$

$\omega x = v \sin\omega t$

$\frac{p}{m} = v\cos\omega t$ $\Big\} \Rightarrow \frac{\omega^2 x^2}{v^2} + \frac{p^2}{m^2 v^2} = 1$ $\quad \frac{2E}{m} \quad \frac{2Em}{2Em}$

Harmonički oscilator:



$$E = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2$$

$$1 = \frac{q^2}{\frac{2E}{m\omega^2}} + \frac{p^2}{2mE}$$

a^2 $\quad b^2$

jba. elipse u faznom prostoru

$\sqrt{2mE \cdot \frac{2E}{m\omega^2}}$

$p(q)$

površina elipse $\quad \oint p\,dq = ab\pi = \frac{2\pi E}{\omega} = \frac{2\pi\, n\hbar\omega}{\omega}$

Planck-ova kvantizacija energije $\quad E = n\hbar\omega \quad \Rightarrow \quad \oint p\,dq = nh$

Povodeći se time:

Somerfeld-Wilson → uvjeti kvantizacije

napomena: smisao obilaženja je logičan

$q_k \uparrow \; p_k \sim \dot{q}_k > 0$

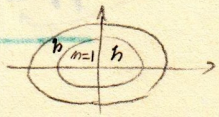
$q_k \downarrow \; p_k \sim \dot{q}_k < 0$

$$\oint p_k\,dq_k = n_k \cdot h \qquad k = 1, 2, 3, \ldots s$$

za sve stupnjeve slobode

→ razlika između susjednih površina je opet h

→ površina se povećava za h



- koristili smo u stat. fizici → ∀ elem. ćelija ima volum. h za s-st. slobode h^s

- ∀ stacionarnom stanju u faznoj ravnini pridružena je ista površina h tj. za s-st. slob. ∀ stac. stanju u faznom prostoru pridružen isti volumen h^s

Liouville - jednako veliki fazni volumeni su jednako vjerojatni $\quad \frac{d\rho}{dt} = 0$

⇒ **3) Bohr-ov postulat**

koju E ima čestica u nekoj točci

sva stacionarna stanja su a priori jednako vjerojatna

tj. ne brinuti još za T i E plina

→ 1915. Stark - u jakom $\vec{E}$ linije H se cijepaju na više drugih

→ Bohr-ova hipoteza: Kružnica nije dovoljna, ∃ čitav niz elipsi sa istom velikom poluosi, pa ćemo za energiju dobiti - isti rezultat jer

Kružnica: $E = -\frac{Ze^2}{2r}$

$$E = -\frac{Ze^2}{2a} \quad *)$$

origin. - ~~a~~ općenito izvedeno na papiru i u slučaju problema dvaju tijela *)'

- a $\vec{E}$ različito djeluje na različite staze (kružnu ili elipsu)

- položaj e^- u gibanju oko jezgre određen je s r, φ (jer sila centralna $\vec{F} = f(r)\cdot\vec{r_0}$)

→ dva kvantna uvjeta

$$\oint p_r\,dr = n_r h \qquad \oint p_\varphi\,d\varphi = n_\varphi h \quad = p_\varphi\, 2\pi$$

$n_r = 0, 1, 2, \ldots$ $\qquad$ $n_\varphi = 1, 2, 3, \ldots$

$p_\varphi = \text{const}$ II Kepl. zakon

za elipsu: $r = \frac{p = a(1-\varepsilon^2)}{-1 \pm \varepsilon\cos\varphi}$ $\quad 0 \le \varepsilon < 1$

$$\Rightarrow \quad p_\varphi = n_\varphi \cdot \hbar$$

n_φ - azimutalni kvantni broj

izvorna Bohr. pretp.

izvedeno na vježbama:

$$-\frac{\mu Z^2 e^4}{2\hbar^2 n^2} = E = -\frac{mZ^2e^4}{2\hbar^2 n^2}$$

glavni kvantni broj

$$n = n_r + n_\varphi$$

n_r - radijalni kvantni broj; n_φ - azimutalni kvantni broj

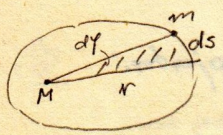
⇓ *)

$r = \frac{n^2\hbar^2}{mZe^2}$

$$\frac{\hbar^2 n^2}{\mu Z e^2} = a = \frac{\hbar^2 n^2}{mZe^2} \qquad n = 1, 2, 3, \ldots$$

↑ jednaka radijusima Bohrovih kružnica, jer ti radijusi daju jedine empiriške vrijednosti (i u slučaju problema 2. tijela)

→ Kvantizacija velike poluosi elipse



$$dP = \frac{1}{2} r\,ds = \frac{1}{2} r^2 d\varphi \qquad p_\varphi = mr^2\dot{\varphi}$$

$$\Big\}\; dP = \frac{p_\varphi}{2m}\,dt \quad \Rightarrow \quad P = \frac{p_\varphi}{2m}\cdot T = ab\cdot\pi$$

II Kepler-ov zakon

$$E = \frac{\mu}{2}(\dot{r}^2 + r^2\dot{\varphi}^2) - \frac{Ze^2}{r} \qquad p_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = \mu r^2\dot{\varphi}$$

III Kepl. zakon $\quad \frac{T^2}{a^3} = \frac{4\pi^2 m}{Ze^2} \overset{\text{točnije}}{=} \frac{4\pi^2 m}{Ze^2}\left(\frac{M}{m+M}\right)$ origin., tada $|\vec{\Pi}| = \mu r^2\dot{\varphi} = p_\varphi = n_\varphi\hbar$ (Const.) $\quad$ iz $\oint p_\varphi d\varphi = n_\varphi h$

$$\frac{T^2}{a^2} = \frac{4\pi^2 m}{Ze^2}\cdot\frac{n^2\hbar^2}{mZe^2}$$

II Kepler-ov $\quad \dot{P} = \frac{C}{2} = \frac{|\vec{\Pi}|}{2\mu} = \frac{p_\varphi}{2\mu} \quad \Rightarrow \quad P = \frac{p_\varphi}{2\mu}\cdot T = ab\pi$

$$\frac{T}{a} = \frac{b\cdot\pi\cdot 2m}{n_\varphi\cdot\hbar}$$

$$b = n_\varphi a\,\frac{T}{a^2}\cdot\frac{\hbar}{2\pi m}$$

$$b = n_\varphi a\cdot\frac{2\pi m\hbar}{Ze^2}\cdot\frac{\hbar}{2\pi m}\cdot\frac{Ze^2}{n^2\hbar^2} = \frac{n_\varphi a}{n}$$

$$\Rightarrow \quad b = a\,\frac{n_\varphi}{n}$$

$\Rightarrow n_\varphi > 0$ inače elipsa degenerira u pravac

$n_\varphi = 1, 2, 3, \ldots$ $\qquad$ $\Rightarrow n > 0$

$n = 1, 2, 3, \ldots$

točnije: $b = a\,\frac{n_\varphi}{n}$ i u slučaju problema 2. tijela

*)' papir

$$\begin{matrix} 3 & 2 & 3 \\ 2 & 1 & 2 \\ 1 & 0 & 1 \end{matrix}$$

$b = a\frac{n_\varphi}{n}$ $\quad n = n_r + n_\varphi$

$n_r = 0 \Rightarrow b = a$ (i=0) kružnica

$n = n_\varphi \quad p_r = 0$ jer $p_r = m\dot{r} = 0$ ($\dot{r}=0$)

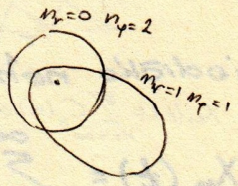
$n = 1 \Rightarrow n_r = 0 \quad n_\varphi = 1$ kružnica

$\oint p_r dr = n_r h = 0$

$\Rightarrow p_r = 0$

$n = 2 \Rightarrow n_r = 0 \quad n_\varphi = 2 \Rightarrow b = a$ kružnica

$n_r = 1 \quad n_\varphi = 1 \Rightarrow b = \frac{a}{2}$ elipsa



$n = 3 \Rightarrow n_r = 0 \quad n_\varphi = 3 \quad b = \frac{3}{3}a$ kružnica

$n_r = 1 \quad n_\varphi = 2 \quad b = \frac{2}{3}a$ elipsa

$n_r = 2 \quad n_\varphi = 1 \quad b = \frac{a}{3}$ elipsa

⋮

Princip Korespodencije

- vazan u Q.M.

- most između Klas. i Q.M., analogno kao $v \ll c$ relativ. $\to$ Klas. Newt.

$\to$ Kvantni zakoni primjenjeni na dovoljno velikim dim. prelazeći Klasične

1° $E_n = -\frac{mZ^2e^4}{2n^2\hbar^2} \qquad r_n = \frac{n^2\hbar^2}{mZe^2} \qquad \omega_n = \frac{v_n}{r_n} = \frac{mZ^2e^4}{n^3\hbar^3}$

r_n raste s n $\to$ koju ν do emitir. atom s velikog n na bliske putanje sebi

$\to$ za $n \gg 1$ E_n gotovo kontinuiran fja. od n $\qquad E_{n+1} - E_n \approx \frac{2n+1}{n^2(n+1)^2} \to 0$

2° prijelaz $n \to n-k \qquad n \gg k > 0 \Rightarrow (n-k) \gg 0 \Rightarrow 0 < \frac{k}{n} \ll 1 \Rightarrow \left|\frac{k}{n}\right| \ll 1$

$$\omega_{nn-k} = \frac{E_n - E_{n-k}}{\hbar} = \frac{mZ^2e^4}{2\hbar^3}\cdot k \cdot \frac{2n-k}{n^2(n-k)^2} = \frac{1}{n(n-k)^2} + \frac{1}{n^2(n-k)} =$$

za $|x|<1$ $\quad \frac{1}{1-x} = 1 + \sum_{n=1}^{\infty} x^n \qquad \frac{1}{(1-x)^2} = 1 + \sum_{n=1}^{\infty}(n+1)x^n$

$$= \frac{1}{n^3}\left[\frac{1}{(1-\frac{k}{n})^2} + \frac{1}{(1-\frac{k}{n})}\right] =$$

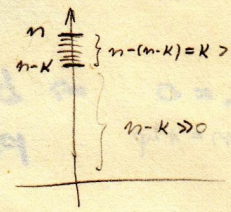
$$= \frac{1}{n^3}\left[2 + \sum_{n=1}^{\infty}(n+2)\left(\frac{k}{n}\right)^n\right] \approx \frac{2}{n^3}$$

$$\omega_{nn-k} = \frac{mZ^2e^4}{\hbar^3 n^3}\cdot k$$

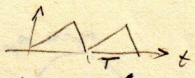
$\overset{n}{(n-k)} \geq 0 \quad \{ n-(n-k) = k$

→ Frekvencija ophoda - Klasična frekvencija staze

$$\omega_n = \omega(n) = \frac{v_n}{r_n} = \frac{m Z^2 e^4}{n^3 \hbar^3} \overset{\text{općenito}}{=} \frac{\mu Z^2 e^4}{n^3 \hbar^3}$$



$$\Rightarrow \quad \omega_{nn-k} = k \cdot \omega(n)$$ - vodilja Bohra, Heisenberga



sila nije $\vec{F} = -k\vec{r}$

→ periodičko neharmoničko gibanje možemo razviti u Fourier. red

slučaj elipse

$$X_n(t) = \sum_{k=-\infty}^{\infty} C_k(n)\, e^{i\left(\frac{2\pi}{T_n(n)}\right) k \cdot t} \qquad \omega(n) = \frac{2\pi}{T_n(n)}$$

i) $$X_n(t) = \sum_{k=-\infty}^{\infty} a_k(n)\, e^{i k \omega(n) t}$$

projekcija na x-os

Kvantna frekv. ω_{nn-k} daje gornje tonove osnovne frekvencije $\omega(n)$ koja je ista za n-tu kružnicu ili elipsu

$$\omega(n) = \frac{2\pi}{T_n}$$

ophodno vrijeme isto za kružnicu ili eliptičnu za isti n

$$T_n = \frac{2\pi n^3 \hbar^3}{\mu Z^2 e^4}$$

- čisto harmoničko gibanje za $k=1$ $\Rightarrow a_1$ tj. $\omega_{nn-1} = \omega(n)$

$k=1$ $\quad X_n(t) = a_1(n) \cdot \left[e^{i\omega(n) t} \right]$

- Korist od principa Korespod.

$|a_k|^2 \sim$ intenzitetu spektralne linije

uz frekv. ω_{nn-k} → vjerojatnost za taj prijelaz a_{nn-k}

$$\omega_{nn-k} = k \cdot \omega(n) \qquad a_{nn-k} = a_k(n)$$ principo Korespodencije

klas. amplituda

3° Bohr - ono što vrijedi za velike kvantne brojeve širi na sve
→ Korespodencija klasičnih i kvantnih veličina

Supek Modifizika 404. 1925. W. Heisenberg napušta opću predodžbu o stazama elektrona u atomu i polazi sa stajališta, da teorija atomnih procesa mora promatrati amplitude i frekv. kao jedino fizički stvarne, ne vezući s tim veličinama klasičnu predodžbu elektronskih staza u atomu.

Mjesto klasičnih frekv. i amplituda, koje se izvode iz Fourierove analize diskretnih klasičnih elektronskih staza, promatra Heisenberg dobivene dvodimenzionalni niz frekvencija ν_{nm} & a_{nm}, koji odgovara prijelazima elektrona iz stacionarnog stanja n u stac. stanje m.

formir. matrica ←

406. U Heisenbergovoj kvantnoj mehanici povezani su elementi matrice u formalno slične zakone kao Fourier-ovi elementi u klasičnoj mehanici. Uz tu formalnu sličnost, uzrokovanu principom Korespodencije, postoji bitna razlika u fizičkom značenju klasičnih i kvantnih veličina.

$X_n(t)$ - je pomak - ito realna veličina $\Rightarrow$ $X_n(t) = X_n^*(t)$ ii) - uvjet realnosti -

Konjug. Kompleks.

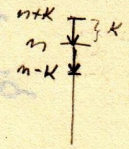
pišem umjesto $k \to -k$

$$X_n^*(t) = \sum_{k=-\infty}^{\infty} a_k^*(n) e^{-ik\omega(n)t} = \sum_{k=-\infty}^{\infty} a_{-k}^*(n) e^{ik\omega(n)t} = \sum_{k=-\infty}^{\infty} a_k(n) e^{ik\omega(n)t}$$

i) & ii) $\Rightarrow$ $\underline{a_{-k}^*(n) = a_k(n)}$ $= a_{nn-k}$

$a^*_{nn-(-k)}$

princip Korresp. $\Rightarrow$ $a_{nn-k} = a^*_{nn+k}$



za $n \gg k \Rightarrow (n-k) \gg 0 \Rightarrow$ nivoi praktički ekvidistantni $\Rightarrow$ svejedno da li $n \to n+k$ ili $n \to n-k$ prijelaz gore ili dolje tj. vise ili niže po energ. razmaci praktički ekvidistantni i ne ovise toliko o $\underline{n}$ tj. $\nu_{n+k\,n} \approx \nu_{n\,n-k}$

pa što vrijedi za frekvencije vrijedi i za amplitude

$$\Rightarrow a_{nn-k} = a^*_{nn+k} = a^*_{n\,n-k\,n}$$

$n-k=m$

$$\Rightarrow \underline{a_{nm} = a^*_{mn}}$$ Kvantni uvjet

→ **Izborna pravila** : - odredjuju kvantnomeh. amplitudu a_{nm}

Ako u klas. Fourier. razvoju i) neki koef. $a_k(n)$ ne dolaze $\xrightarrow[\text{Korresp.}]{\text{princip.}}$ te veličine ne dolaze ni u kvantnom slučaju, dakle preko principa Korresp. zaključ. o izbornim pravilima tj. nalazimo koji su prijelazi dozvoljeni a koji zabranjeni !

Ilustracija :

1) Harmonički oscilator

$E_n = n\hbar\omega$ $\qquad \omega_{nn'} = \frac{E_n - E_{n'}}{\hbar} = \underbrace{(n-n')}_{k}\omega$ $\qquad n' = n-k \Rightarrow n-n' = k$

da li se tu pojavljuje sve frekv.

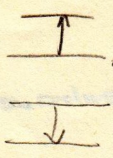
→ čisto harmonisko gibanje $\Rightarrow$ Klas. Fourier. razvoju 1 frekv. i to ω i u kvantnom slučaju $k=1$

$k=1$ & $k=-1$ $\xrightarrow[\text{Korresp.}]{\text{princip}}$

$$\left.\begin{aligned} x(t) &= a_1(n) e^{i\omega(n)t} + a_{-1}(n) e^{-i\omega(n)t} \\ \| \\ x^*(t) &= a_1^*(n) e^{-i\omega(n)t} + a_{-1}^*(n) e^{i\omega(n)t} \end{aligned}\right\} \Rightarrow$$

$\Rightarrow a_1(n) = a_{-1}^*(n) \Rightarrow a_{nn-1} = a^*_{nn-(-1)} = a^*_{n\,n+1}$

$\Rightarrow$ samo 2 slučaja (prijelaza) $n' = n+1$, $n' = n-1$

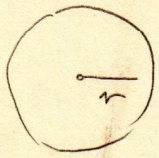


apsorbcija $a^*_{n\,n+1}$

emisija $a_{n\,n-1}$

$\rightarrow$ emisije i apsorbcije gdje se kvantni broj n mijenja za 1, 3, ... ne 3 za harmon. oscilator

2) Rotator



$\Rightarrow p_r = m\dot{r} = 0$

$r = const. \Rightarrow n_r = 0$ $\quad \oint p_r dr = n_r h \quad \Rightarrow n = n_\varphi$

čisto harmonijsko kretanje $\rightarrow \Delta n = \pm 1 \rightarrow \Delta n_\varphi = \pm 1$

– u stat. fizici 2-A molekule rotatori

općenito: 2-A molek. $M = m_1 + m_2$ $\quad \mu = \frac{m_1 m_2}{M}$

$E_K = \frac{p^2}{2M}$ (trans.) $+ \frac{p^2}{2\mu}$ (rel. transl.)

$p^2 = p_r^2 + \frac{1}{r^2}\left(p_\vartheta^2 + \frac{1}{\sin^2\vartheta} p_\varphi^2\right)$

$p_r = \mu\dot{r} = 0$

$p_\vartheta = \mu r^2 \dot{\vartheta} = 0$ rotatori rotacija u jednoj ravnini

$p_\varphi = \mu r^2 \sin^2\vartheta\, \dot{\varphi}$ ne mora biti

rotac. energija 2-A molek. $E_{rot} = \frac{1}{2\mu}\frac{1}{r^2} p_\varphi^2$

$$E_{rot} = \frac{M^2}{2J} = \frac{n_\varphi^2 \hbar^2}{2J} = \frac{n^2\hbar^2}{2J} \quad \text{jer } n = n_\varphi$$

$J = \mu r^2$

$\vec{M} = \vec{r} \times \vec{p}$ angularni moment

$M = p_\varphi = n_\varphi \hbar$ (Bohr teor.)

napomena: pitanje je da li postoji takav idealan sistem – rotator da je $p_\varphi = const.$ $\Rightarrow J$ je sila centralna

$$\omega_{nn'} = \frac{E_n - E_{n'}}{\hbar}$$

$(n-k)$ $\quad k = \pm 1$

čista rotacija $\rightarrow$ harmonij. kretanje $\Rightarrow n' = n \pm 1$

jer gibanje po kružnici samo osnovni ton

emisija: $n \rightarrow n-1$

$$\omega_{nn-1} = \frac{\hbar}{2J}\left[n_\varphi^2 - (n_\varphi - 1)^2\right] = \frac{\hbar}{J}\left(n_\varphi - \frac{1}{2}\right)$$

to bi trebalo biti pravilo za emitiranje frekv. 2-A molek.

– exp: daju dosta dobro slaganje

$\rightarrow$ potpuno slaganje ako se promijeni Bohr-ov uvjet kvantizacije

$$M^2 = p_\varphi^2 = \hbar^2 l(l+1) \quad l = 0, 1, 2, 3, \ldots \quad \text{inače } p_\varphi = n_\varphi \hbar \quad n_\varphi = 1, 2, 3, \ldots$$

$l^2 + l - l(l-1) = l^2 l - l^2 + l$

$$\Rightarrow E_l = \frac{\hbar^2 l(l+1)}{2J} \quad \Rightarrow \omega_{l\,l-1} = \frac{\hbar}{J} \cdot l$$

u potp. suglasnosti s exp.

suvišna je bila ona $\frac{1}{2}$ $\rightarrow$ kasnije kako dokaz. dotih korektura

Heisenberg-ova teorija

1) Bohr-ova korekcija s kružnom elipsom ne daje dovoljan broj stanja s istom energijom u odnosu na linije $n = n_r + n_\varphi$ $\quad \underbrace{n_r = 0, 1, \dots n-1}_{n \text{ stanja}}$ $\quad n_\varphi = n, n-1, \dots 1$

Bohr $\rightarrow n$

Pokazuje se da je broj kvantnih stanja iste energije u H $\rightarrow 2n^2 > n$

2) Bohr-ova teorija na He ne daje dobre rezultate
- čisto dva operativna nedostatka

3) u Bohr-ovoj teoriji radimo s pojmom staze $\rightarrow$ u t času bi znali p, r

$\rightarrow$ relacije neodređenosti - ne znače lom klas. fizike

$$\Delta r \cdot \Delta p \approx h$$

- dominantno za područje gdje je h relativno veliko

H-atom

$r \simeq 10^{-8}$ cm

$v = 10^8$ cm/s $\quad m = 10^{-27}$ g $\quad \Rightarrow p = 10^{-19}$ cgs

$\Big\}$ $r \cdot p = 10^{-8} \cdot 10^{-19} = 10^{-27} \approx h$ - upravo produkt neodređen

$\rightarrow$ informacije Bohr-ove teorije o stazi su bezvrijedne - sve rezultate uzimamo soprezom

s rezervom prema starom kvantnoj teoriji

1924. Heisenberg - Schrödinger - nova kvantna teorija

ono što exp. zaznajemo su frekvencije, dakle nivoi $E_0, E_1, E_2, \dots$ i intenziteti spektralnih linija

	E_0	E_1	E_2	...
E_0	$\omega_{00} = 0$, a_{00}	ω_{01}, a_{01}	$\omega_{02} = \frac{E_0 - E_2}{\hbar}$, a_{02}	
E_1	ω_{10}, a_{10}	$\omega_{11} = 0$, a_{11}	ω_{12}, a_{12}	
E_2	$\omega_{20} = \frac{E_2 - E_0}{\hbar}$, a_{20}	ω_{21}, a_{21}	$\omega_{22} = 0$, a_{22}	
$\vdots$				

Poznavanjem kvantnih amplituda i frekvencija uglavnom je iscrpeno naše znanje o atomu.

Heisenberg pok. izgr. kvantne meh. polazeći od te sheme.

Osnovna ideja Heisenbergove mehanike matrica, koja je nastala dosljednom primjenom principa korespondencije na atomne procese.

str. 406

Neodrživost klasične predodžbe staze u atomnim dimenzijama, a kvalitativno slaganje izmedu klasičnih Fourier-ovih elemenata i empiričkih kvantnih frekvencija i amplituda, navelo je Heisenberga na misao, da za kvantne veličine ω_{nm}, a_{nm} vrijede slični zakoni kao za klasične Fourier-ove elemente, ali da se te kvantne veličine ne smiju rezati uz zorne predodžbe staza. U atomnoj fizici treba da više mislimo na same Fourier-ove elemente, a da ih pri tom ne povezujemo u stazu elektrona. Fourier-ovi elementi nastupaju kao samostalne fizičke veličine, a njihovo fizičko značenje očituje se u emitiranoj svjetlosti.

$X_n(t) = \sum_{m=-\infty}^{\infty} X_{nm}$ – projekcija na x-os svih mogućih periodičkih klasičnih gibanja poelipsama

uvedimo veličine

$$X_{nm} = a_{nm} e^{i\omega_{nm} t}$$

Klas. slaži $x \xrightarrow{\text{korresp.}}$ matrica X
Kartezij. koord.

sveukupnost veličina

sveukupnost tih veličina u kvadratnoj shemi

$$X = \begin{pmatrix} X_{00} & X_{01} & \cdots \\ X_{10} & X_{11} & \cdots \\ & & \ddots \end{pmatrix}$$

impuls

$$p = \begin{pmatrix} p_{00} & p_{01} & \cdots \\ p_{10} & p_{11} & \cdots \\ \vdots & & \end{pmatrix}$$

jer $p = m\dot{x}$

i za ostale veličine ovisne o p, x

→ pitanje algebre koju zadovoljavaju te veličine

→ matrična algebra

$\omega_{nm} = -\omega_{mn}$ jer $\omega_{nm} = \frac{E_n - E_m}{\hbar} = -\frac{E_m - E_n}{\hbar} = -\omega_{mn}$

$a_{nm} = a^*_{mn}$ – konjugiran $\quad X_{nm} = a_{nm} e^{i\omega_{nm} t}$ $\Rightarrow X^*_{nm} = a^*_{nm} e^{-i\omega_{nm} t} = a_{mn} e^{i\omega_{mn} t}$

$\Rightarrow \underline{X^*_{nm} = X_{mn}}$ – konjug. **Hermitske matrice** (tj. hermitski simetrične) $A^* = A \quad A^* = \bar{A}'$

$\bar{X}_{nm} = X_{mn}$ (*) $\quad X = [(X_{nm})_{nm}] \Rightarrow X^* = [(\bar{X}_{nm})_{mn}] \overset{(*)}{=} [(X_{mn})_{mn}] = X$

→ još kvantni uvjeti – u staroj kvantnoj teoriji $p_q = n_q \hbar$ iz Somerfeld. $\oint p_k dq_k = n_k \hbar$

Heisenberg: pokazuje da se stari kv. uvjeti mogu napisati u novom obliku

$$\underline{-\sum_l \omega_{nl} |a_{nl}|^2 = \frac{\hbar}{2M}}$$

sva moguća stanja atomnog sustava – masa prom. čestice

→ Supek II 16,17

može se pokazati da slijedi iz:

$[q_i, p_j] = i\hbar\delta_{ij}$ $\quad pX - Xp = \frac{\hbar}{i}$ $\quad$ tj. $[p, x] = \frac{\hbar}{i} \cdot I$

opć. matrice

može se izvesti iz Somerfeld. Wilson uvjeta kvantizacije Supek II 17.

za matrice narušena komutativnost za $\frac{\hbar}{i}$

1- II $[p, x] = \frac{\hbar}{i}$

most prema klas. fizici kad p i x komutiraju

(*) $\hbar \to 0 \Rightarrow px = xp$

1- II **Harmonički oscilator** - odred. energ. spektar iz tih komut. svojstava

$$\ddot{X} = -\omega_0^2 X \quad \text{- matrica}$$

$$\ddot{X}_{nm} = -\omega_0^2 X_{nm} \qquad X_{nm} = a_{nm} e^{i\omega_{nm} t}$$

$$-a_{nm}\omega_{nm}^2 \cancel{e^{i\omega_{nm}t}} = -\omega_0^2 a_{nm} \cancel{e^{i\omega_{nm}t}} \qquad \ddot{X}_{nm} = -a_{nm}\omega_{nm}^2 e^{i\omega_{nm}t}$$

$\neq 0$

$$a_{nm} \cdot (\omega_{nm}^2 - \omega_0^2) = 0 \quad (*) \quad \Rightarrow \omega_{nm} = \pm\omega_0$$

$\omega_{nn} = 0 \Rightarrow a_{nn} = 0$

$\downarrow$ m/n vjerojatnost prijelaza iz n-tog u m-to kvantno stanje (*)

$$\ddot{X} = -\omega_0^2 X \Rightarrow X(t) = a_{-1} e^{-i\omega_0 t} + a_1 e^{i\omega_0 t}$$

princip korespondencije: samo oni prijelazi gdje $m = n \pm 1$ $a_{nm} \neq 0$

$$\omega_{nm-k} = k\,\omega(n) = k\omega_0 \Rightarrow \begin{cases} \omega_{nn-1} = \omega_0 & \text{emisija} \quad \downarrow \\ \omega_{nn+1} = -\omega_0 & \text{apsorbcija} \quad \uparrow \end{cases}$$

u skladu s (*)

$$a_{nm} = 0 \quad \text{za } m \neq n \pm 1$$

→ korištenje komutacionih pravila (vježbe 5.)

(*) $a_{nm} = a_{mn}^*$
a za realne $a_{nm} = a_{mn}$

$$a_{nn+1} \overset{(*)}{=} a_{n+1n} = \sqrt{\frac{\hbar}{2M\omega_0}} \cdot \sqrt{n+1}$$

masa čestice

(*) impuls: $p_{nm} = M \frac{d}{dt} x_{nm}$

$$H = \frac{p^2}{2M} + \frac{M\omega_0^2}{2} x^2 = \frac{\hbar\omega_0}{2} \begin{pmatrix} 1 & & & 0 \\ & 3 & & \\ & & 5 & \\ 0 & & & 7 \ldots \end{pmatrix}$$

pravilo mat. množenja

$$H_{nm} = \frac{\hbar\omega_0}{2}(2n+1)\delta_{nm} \qquad n = 0, 1, 2, \ldots$$

→ potvrđuje Planck-ovu hipotezu $E_n = \hbar\omega_0 n$ do na $\frac{\hbar\omega_0}{2}$ osnovnog stanja → u vezi s relacijama neodređenosti. Born: 399, 401, 471

$\frac{5\hbar\omega_0}{2}$

$\hbar\omega_0$

$\frac{3\hbar\omega_0}{2}$

$\hbar\omega_0$

$\frac{\hbar\omega_0}{2} \neq 0$

dakle najniže energetsko stanje $\neq 0$

naime: kad bi najniže energ. stanje bilo $= 0$, tada bi x & p bili točno određeni

Algebra Komutatora

$$[A,B] = AB - BA$$

Kvantne veličine $\hat{u}, \hat{v}$ matrice

$$[\hat{u},\hat{v}] = i\hbar \{u,v\}_{q,p} \quad (*)$$

$$= i\hbar \sum_{j=1}^{s} \left(\frac{\partial u}{\partial q_j}\frac{\partial v}{\partial p_j} - \frac{\partial u}{\partial p_j}\frac{\partial v}{\partial q_j} \right)$$

$$[A \pm B, C] = (A \pm B)C - C(A \pm B) =$$

$$= [A,C] \pm [B,C]$$

$$[C, A \pm B] = -[A \pm B, C] = -[A,C] \mp [B,C] = [C,A] \pm [C,B]$$

$$[AB, C] = (AB)C - C(AB) + ACB - ACB =$$

$$= A[B,C] + [A,C]B$$

$$[C, AB] = A[C,B] + [C,A]B$$

1-D slučaj

matrice

$$[p, q] = \frac{\hbar}{i}\frac{\partial q}{\partial q} I \quad (*)' = \frac{\hbar}{i}\frac{\partial p}{\partial p} \cdot I$$

i tvrdimo da je poopćenje za proizv. fju. $F(q,p)$

$$[p, F] = \frac{\hbar}{i}\frac{\partial F}{\partial q} \qquad (*)' \quad [F, q] = \frac{\hbar}{i}\frac{\partial F}{\partial p} \quad (*)$$

$$(*) \Rightarrow \quad [p,F] = i\hbar \{p,F\}_{q,p} = i\hbar \left(\underbrace{\frac{\partial p}{\partial q}}_{0}\frac{\partial F}{\partial p} - \frac{\partial p}{\partial p}\frac{\partial F}{\partial q} \right) = -i\hbar \frac{\partial F}{\partial q}$$

dokaz indukcijom: 1° $F = q, p$ prijašnji slučaj 2- gradimo kompliciran. fje. zbrojevima i produktima

$$\dot{p} = -\frac{\partial H}{\partial q} = \{p,H\} \qquad \dot{q} = \frac{\partial H}{\partial p} = \{q,H\}$$

$$\text{općenito } \frac{dF}{dt}(q_j, p_j, t) = \frac{\partial F}{\partial t} + \{F,H\} \quad (*) \quad j=1,\dots,s$$

$$[\hat{q}_i, \hat{p}_j] = \hat{q}\hat{p} - \hat{p}\hat{q} = i\hbar \underbrace{\{q_i, p_j\}}_{\delta_{ij}} = i\hbar\,\delta_{ij}$$

$$\frac{d}{dt}F(q,p) = \{F,H\}$$

F_1 & F_2 koje zadovoljavaju pravila $(*)$

$\forall$ fju $F(q,p)$ možemo razviti u red zbrojeva produkata q & p koji zadovolj. $(*)'$ tako da je $(*)$ dokazano

$$[p, F_1 + F_2] = \underbrace{[p, F_1]}_{\frac{\hbar}{i}\frac{\partial F_1}{\partial q}} + \underbrace{[p, F_2]}_{\frac{\hbar}{i}\frac{\partial F_2}{\partial q}} = \frac{\hbar}{i}\frac{\partial}{\partial q}(F_1 + F_2)$$

$$[p, F_1 F_2] = F_1 \underbrace{[p, F_2]}_{\frac{\hbar}{i}\frac{\partial F_2}{\partial q}} + \underbrace{[p, F_1]}_{\frac{\hbar}{i}\frac{\partial F_1}{\partial q}} F_2 = \frac{\hbar}{i}\frac{\partial}{\partial q}(F_1 F_2)$$

analogno: $[F_1 + F_2, q]$ & $[F_1 F_2, p]$

$F(q,p)$ rastavimo u red i provjerimo član po član

specijalno: $F = H(q,p)$

$$\frac{\partial H}{\partial q} = \frac{i}{\hbar}[p,H] \qquad \frac{\partial H}{\partial p} = \frac{i}{\hbar}[H,q]$$

Kanonske jbe.: $\frac{dq}{dt} = \frac{\partial H}{\partial p}$ $\quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}$

$$\Rightarrow \frac{dq}{dt} = \frac{i}{\hbar}[H,q] \qquad \frac{dp}{dt} = \frac{i}{\hbar}[H,p] \qquad (**)'$$

ponovimo postupak: pretp. F_1 i F_2 zadovolj. pravila

$$\frac{i}{\hbar}[H,F_1+F_2] = \underbrace{\frac{i}{\hbar}[H,F_1]}_{\frac{dF_1}{dt}} + \underbrace{\frac{i}{\hbar}[H,F_2]}_{\frac{dF_2}{dt}} = \frac{d}{dt}(F_1+F_2)$$

$$\frac{i}{\hbar}[H,F_1F_2] = \frac{i}{\hbar}F_1[H,F_2] + \frac{i}{\hbar}[H,F_1]F_2 = F_1\frac{dF_2}{dt} + \frac{dF_1}{dt}\cdot F_2 = \frac{d}{dt}(F_1\cdot F_2)$$

$F(q,p)$ razložimo u red potencija od q,p (za njih je ispunjeno $(**)'$) i provjerimo član po član

vremen. derivacija matrice F

$$\Rightarrow \frac{dF(q,p)}{dt} = \frac{i}{\hbar}[H,F]_{Q.M.} \qquad (**)$$

jba. gibanja za $F(q,p)$

$$\text{općenito} \quad \frac{dF(q,p,t)}{dt} = \frac{i}{\hbar}\underbrace{[H,F]}_{i\hbar\{H,F\}} + \frac{\partial F}{\partial t} \qquad \text{za } F(q,p,t)$$

$$= -\{H,F\} + \frac{\partial F}{\partial t} = \{F,H\} + \frac{\partial F}{\partial t} \quad \text{klasično}$$

Veza s Poisson-ovim zagradama:

$$\{F_1,F_2\}_{q,p} = \sum_{k=1}^{s} \frac{\partial F_1}{\partial q_k}\frac{\partial F_2}{\partial p_k} - \frac{\partial F_1}{\partial p_k}\frac{\partial F_2}{\partial q_k} \qquad F_1, F_2 \text{ matrice}$$

$F(q,p)$

$$\frac{dF(q,p)}{dt} = \{F,H\} = \sum_{k=1}^{s} \frac{\partial F}{\partial q_k}\underbrace{\dot{q}_k}_{\frac{\partial H}{\partial p_k}} + \frac{\partial F}{\partial p_k}\underbrace{\dot{p}_k}_{-\frac{\partial H}{\partial q_k}}$$

$\Rightarrow$ sličnost nije povrćna, već proizlazi iz duboke korespondencije između klas. i kvantnih veličina

$$\{F_1,F_2\} \to \underbrace{-\frac{i}{\hbar}}_{\frac{1}{i\hbar}}[F_1,F_2]$$

klasični komutator

Supek II 40.

vrijednosti Poissonovih zagrada od koordinata i konjugiranih impulsa u klas. teoriji

$$\{q_k,q_l\} = 0 \qquad \frac{1}{i\hbar}[q_k,q_l] = \frac{1}{i\hbar}(q_kq_l - q_lq_k) = 0$$

$$\{p_k,p_l\} = 0 \quad !!! \quad \to \quad \frac{1}{i\hbar}[p_k,p_l] = 0$$

$$\{q_k,p_l\} = \delta_{kl} \qquad \frac{1}{i\hbar}[q_k,p_l] = \delta_{kl}$$

To su osnovna komutacijska pravila kvantne meh. Iako je u klasičnoj mehanici sadržan korijen, zašto q_k i p_k ne da komutiraju u kvantnoj teoriji. Prema tome je posve prirodno, da klasične Poiss. zagrade zamijenimo uvedenim komutacionim izrazima. Obzirom da je ta koresp. ispunjena za q_k, p_k, bit će zbog izvodbe algebre ispunjena i za složenije izraze.

Poissonove zagrade predstavljaju prirodno izbačite za prijelaz od klasične na kvantnu mehaniku.

Specijalno: $F = H$ ako H neovisi o t expl.

$$\Rightarrow \frac{dH}{dt} = \frac{i}{\hbar}[H,H] = 0 \qquad \Rightarrow \text{matrica } H \text{ je konstanta gibanja}$$

$$x_{nm} = a_{nm} e^{i\omega_{nm} t} \qquad \omega_{nn} = 0 \Rightarrow x_{nn} = a_{nn}$$

$\Rightarrow$ mišao: H ima samo dijagonalne elemente jer oni jedino neovise o t

Postuliramo: $H_{nm} = E_n \delta_{nm}$ H dijagonalna matrica

(par bi valjalo biti i O matrica)

energ. stac. stanja – opravdanje: što odatle neposredno proizlazi: Ritz-Bohrov princip o frekvencijama spektralnih linija

motivacija: $\frac{dH}{dt} = 0$ $\quad x_{nm} = a_{nm} e^{i\omega_{nm} t}$

Supek II 23

Born-Jordan-Heisenberg matrična formulacija:

1) $[p_k, q_l] = \frac{\hbar}{i}\delta_{kl} \quad [p_k, p_l] = 0 \quad [q_k, q_l] = 0$

2) $H_{nm} = E_n \delta_{nm}$ tj. dijagon. matrica H, sa energ. stac. stanjima na dijagonali

$\rightarrow$ iz jbe. gibanja $\frac{dF(q,p)}{dt} = \frac{i}{\hbar}[H,F]$ $\quad HF - FH$ $\quad F(q,p)$ – matrična f-ja. koja ne ovisi expl. o t

$F_{(q,p)} = [(F_{nm}(q,p))_{nm}]$

$$\frac{d}{dt} F_{nm}(q,p) = \frac{i}{\hbar}(HF)_{nm} - \frac{i}{\hbar}(FH)_{nm} =$$

$$= \frac{i}{\hbar}\sum_{l=0} (\underbrace{H_{nl}}_{E_n\delta_{ln}} F_{lm} - F_{nl} \underbrace{H_{lm}}_{E_m\delta_{lm}})$$

$$= \frac{i}{\hbar} F_{nm} \underbrace{(E_n - E_m)}_{\text{po Bornu}}$$

$$\omega_{nm} = \frac{E_n - E_m}{\hbar}$$

$$\Rightarrow \frac{d}{dt} F_{nm} = i\omega_{nm} F_{nm}(q,p) \Rightarrow \frac{d}{dt} F_{nn} = 0$$

$\frac{dF_{nm}}{F_{nm}} = i\omega_{nm}\, dt$

$\ln F_{nm} = i\omega_{nm} t + \ln C$

$F_{nm} = C e^{i\omega_{nm} t}$

$F_{nm}(q(0), p(0)) = C \cdot 1$

$\Rightarrow$ proizvoljna fizikalna veličina – matrica s vrem. konstantnim na dijagonali, ali drugdje nisu vrem. konstante

$$F_{nm}(t) = \overbrace{F_{nm}(0)}^{f_{nm}} e^{i\omega_{nm} t}$$

– taj oblik matričnih elemenata proizlazi iz činjenice da je H dijagon. matrica

!!!

zapravo

$$F_{nm}(q(t), p(t)) = F_{nm}(q(0), p(0)) e^{i\omega_{nm} t}$$

jer izgleda kao da F_{nm} ovisi expl. o t množitelj faktor $e^{i\omega_{nm} t}$ se odnosi na koordinate q koje ga sadržavaju

Problem angularnog momenta (Kasnije na drugi način)

$$\vec{M} = \vec{r} \times \vec{p} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

Kretanje u sferno sim. potencijalu $U(\vec{r})$ (*)

$\vec{M} = \vec{C}$ Konstanta gibanja $\Rightarrow M_x, M_y, M_z$ Konst. gibanja (*)'

- sačuvano i u kvan. fizici (Koresp. Poisson. zagr. i Komutatora Konst. mat.)

$$0 \overset{(*)}{=} \frac{d\vec{M}}{dt} = \frac{i}{\hbar}\underbrace{[H, \vec{M}]}_{=0} \Rightarrow 0 \overset{(*)}{=} \frac{dM_x}{dt} = \frac{i}{\hbar}\underbrace{[H, M_x]}_{=0} = \frac{i}{\hbar}[H, yp_z - zp_y] =$$

matrica takoder; ciklički; matrice

$\Rightarrow$ dakle u slučaju centralnih sila moment impulsa komutira sa H.

Kako izgleda ta vrem. konstanta

- pitanje kvantizacije?

$$M_x = y p_z - z p_y$$
$$M_y = z p_x - x p_z$$
$$M_z = x p_y - y p_x$$

Sipak: 25.

$F(q,p) = C \Rightarrow [H, F] = 0 \quad HF = FH$ tj. F komutira sa H

$$(HF)_{nm} = (FH)_{nm}$$

$$\sum_l (\underbrace{H_{nl}}_{E_n\delta_{ln}} F_{lm} - F_{nl} \underbrace{H_{lm}}_{E_m\delta_{lm}}) = 0 \Rightarrow (E_n - E_m) F_{nm} = 0$$

H nedegenerir. dij. matrica tj. $n \neq m \Rightarrow E_n \neq E_m$

(*) $\Rightarrow F$ djag. matrica $\Rightarrow F_{nm} = 0$

obrat: $F_{nm} = F_n \delta_{nm} \Rightarrow (E_n - E_m) F_n \delta_{nm} = 0$ $\quad (E_n - E_m) = 0$

$\Rightarrow (HF)_{nm} = (FH)_{nm} \Rightarrow \frac{dF}{dt} = 0$

$F_{(q,p)} = C$

H degenerir. dij. matrica

$$\begin{pmatrix} E_1 & & & & \\ & E_2 & & & \\ & & E_2 & & \\ & & & E_2 & \\ & & & & E_2 \end{pmatrix} \Rightarrow F = \begin{pmatrix} F^{(1)} & & 0 \\ & F^{(2)} & \\ 0 & & F^{(3)} \end{pmatrix}$$

submatrice koje su dijagonalne – skalarne

submatrice $F^{(r)}$ ne moraju biti dijagonalne

npr. $E_2 = E_3 = E_4 = E_5 \not\Rightarrow F_{nm} \neq 0$ $\quad n = 2,3,4,5$; $m = 2,3,4,5$

∀ dijagonalna matrica je konst. gibanja

ali ∀ konst. gibanja nije dijag. matrica

$$[M_x, M_y] = -\frac{\hbar}{i} M_z = i\hbar M_z$$

$$[M_y, M_z] = -\frac{\hbar}{i} M_x$$

$$[M_z, M_x] = -\frac{\hbar}{i} M_y$$

$M_z = M_x - M_x M_z$

pogledaj i popini KEII – multipolni e.

matrice

$$M_x M_y - M_y M_x = (yp_z - zp_y)(zp_x - xp_z) - (zp_x - xp_z)(yp_z - zp_y) =$$
$$= y p_z z p_x - z p_y z p_x - y p_z x p_z + z p_y x p_z - z p_x y p_z + x p_z y p_z + z p_x z p_y - x p_z z p_y =$$
$$= y p_x p_z \cdot z - \cancel{z p_x z p_y} - \cancel{x p_z y p_z} + x p_y z p_z - y p_x z p_z + \cancel{x p_z y p_z} + \cancel{z p_x z p_y} - x p_z z p_y$$
$$= y p_x p_z \cdot z - x p_z z p_y - y p_x z p_z + x p_y z p_z$$
$$= y p_x p_z \cdot z - x p_y p_z \cdot z - y p_x z p_z + x p_y z p_z$$
$$= (x p_y - y p_x)(z p_z - p_z \cdot z) = M_z \cdot \left(-\frac{\hbar}{i}\right)$$

Koristimo:

$[p_k, q_l] = \frac{\hbar}{i}\delta_{kl}$

$[q_k, q_l] = 0$

$[p_k, p_l] = 0$

postepenom primjenom; komut. svojstva

$\Rightarrow$ Komponente momenta impulsa ne mogu biti istovremeno dijagonalne matrice, najviše može biti jedna od njih

dokaz: Neka M_x dijagonalna, protip. M_y dijagonalna $\Rightarrow M_z = 0 \Rightarrow M_x = 0, M_y = 0$ apsurd tj. trivijalan skup

dijag. matrice komutativne

$A = [(a_n \delta_{nl})_{nl}]$

$B = [(b_m \delta_{lm})_{lm}]$

$$\Rightarrow A \cdot B = [(\sum_l a_n \delta_{nl} b_m \delta_{lm})_{nm}] = [(a_n b_m \delta_{nm})_{nm}]$$
$$B \cdot A = [(\sum_k b_m \delta_{mk} a_n \delta_{kn})_{mn}] = [(b_m a_n \delta_{mn})_{nm}] \quad (=)$$

$$\left.\begin{aligned}[M^2, M_x] &= 0\\ [M^2, M_y] &= 0\\ [M^2, M_z] &= 0\end{aligned}\right\} \quad (**)$$

$$[M^2, M_x] = [M_x^2 + M_y^2 + M_z^2, M_x] = [M_x^2, M_x] + [M_y^2, M_x] + [M_z^2, M_x] =$$

$$= M_x \underbrace{[M_x, M_x]}_{=0} + \underbrace{[M_x, M_x]}_{=0} M_x + M_y [M_y, M_x] + [M_y, M_x] M_y +$$

$$+ M_z [M_z, M_x] + [M_z, M_x] M_z = \cancel{M_y \cdot \frac{\hbar}{i} \cdot M_z} + \cancel{\frac{\hbar}{i} M_z \cdot M_y} + \cancel{M_z \left(-\frac{\hbar}{i}\right) M_y} - \cancel{\frac{\hbar}{i} M_y M_z}$$

$$= 0$$

$$\frac{dM^2}{dt} = \frac{i}{\hbar}[H, M^2] = \frac{i}{\hbar}[H, M_x^2 + M_y^2 + M_z^2] = \frac{i}{\hbar}\left([H, M_x^2] + [H, M_y^2] + [H, M_z^2]\right) =$$

$$= \frac{i}{\hbar}\left(\underbrace{[H, M_x]}_{=0\ (**)} M_x + H \underbrace{[M_x, M_x]}_{=0}\right) = 0$$

M^2 je konstanta gibanja & (**) ne prijeđi da bude dijag., već se slaže ako je još koja komponenta dij. matrica

M^2 može biti dijagonalna matrica, naime kad ne bi M^2 bila const. gibanja nebi smjela biti ni dijagonalna, jer ∀ dij. matrica je konst. gibanja

izaberimo: M_z dijagonalna

M^2 dijagonalna

može se pokazati:

$$M^2 = \hbar^2 l(l+1) \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & \ddots & \\ 0 & & & 1 \end{pmatrix} \quad (*)$$

$$E = [(\delta_{nm})_{nm}]$$

$$(M^2)_{nm} = \hbar^2 l(l+1)\,\delta_{nm}$$

l – angularni kvantni broj

$$M_z = \hbar \begin{pmatrix} l & & & & 0 \\ & l-1 & & & \\ & & l-2 & & \\ & & & \ddots & \\ 0 & & & & -l+1 \\ & & & & & -l \end{pmatrix}$$

$$(M_z)_{nm} = \hbar m\,\delta_{nm}$$

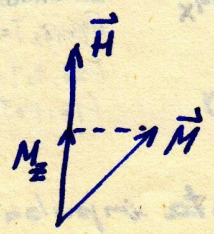
m – magnetski kvantni broj (odgovara si)

$$m = \underbrace{-l, \ldots +l}_{2l+1 \text{ vrij.}}$$

l – angularni kvantni broj

m – magnetski kvantni broj

tj. koje su vrijednosti projekcija $\vec{M}$ na magnetsko polje $\vec{H}$



$l = 0, 1, 2, 3, \ldots$ – odgovara orbitalnim stanjima (Schröd. jba.)

tj. slici od koje smo pošli $\vec{M} = \vec{r} \times \vec{p}$

$l = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ – sistem ima unutarnje stupnjeve slobode — spin

spin

→ spin – unutarnji moment koji može biti i gibanj.

spin – ne možemo interpretirati u analogiji s planetnim modelom e nije kuglica koja bi rotirala oko sebe!

Supek II 31.

7. Teorija transformacije

matričnom računu očigledno značenje

- matrice interpretiramo kao tenzore u n-dim. Hilbert-ovom prostoru
- prostor koji ima toliko koordinata, koliki je stupanj kvadratne matrice (tj. koliko ima redova ili stupaca)
- broj elemenata konačan, ali se sva razmatranja mogu protegnuti i na ∞ matrice
- u tom je prostoru X neki vektor x određen s n-komponenata

$$x \equiv (x_1, \dots x_n)$$ i komponente mogu biti kompleksni brojevi

→ pri afinoj (npr. rot. – tj. pomaci točkastog (Afinog) prostora) transformaciji prostora poprima vektor u novom koord. sistemu komponente određene transf. formulama.

baza: $B = \{e_1, \dots e_n\} \xrightarrow{T} B' = \{e_1', \dots e_n'\}$ $(\ ) = (\ )(\ )^{\perp}$ $B' = B \cdot T^{\perp}$

$e_n' = \sum_m t_{nm} \cdot e_m$

$(\ ) = (\ )(\ )$

$T = [(t_{nm})_{nm}]$ $X = X' \cdot T$ $x_n = \sum_m t_{nm} x_m'$

$A = (T^{-1})^{\perp} = [(a_{nm})_{nm}]$ $X' = X \cdot T^{-1} = X \cdot A^{\perp}$ $x_n' = \sum_m a_{nm} x_m$ ili $X' = A \cdot X^{\perp}$ $(\ ) = (\ A\ )(\ )$

$(\ ) = (\ )(A)^{\perp}$

$B' = \{e_1', \dots e_n'\} \xrightarrow{\tau} B'' = \{e_1'', \dots e_n''\}$ $B'' = B' \cdot \tau^{\perp}$

$\tau = [(\tau_{nm})_{nm}]$ $X' = X'' \cdot \tau$ $x_n' = \sum_m \tau_{nm} x_m''$

$B = (\tau^{-1})^{\perp} = [(b_{nm})_{nm}]$ $X'' = X' \cdot \tau^{-1} = X' \cdot B^{\perp}$ $x_n'' = \sum_m b_{nm} x_m'$ ili $X'' = B \cdot X'^{\perp}$ $(\ ) = (\ B\ )(\ )$

$(\ ) = (\ )(B)^{\perp}$

$$x_n'' = \sum_m b_{nm} \sum_l a_{ml} x_l = \sum_l x_l \sum_m b_{nm} a_{ml} = \sum_l (B \cdot A)_{nl} x_l$$ $X'' = B \cdot A \cdot X^{\perp}$

transformacione formule preglednu u tenzorskoj simbolici

$$\vec{X}' = A \cdot \vec{X} \qquad \vec{X}'' = B \cdot \vec{X}' \qquad \vec{X}'' = B \cdot A \cdot \vec{X}$$

- jedna od najvažnijih operacija je skal. produkt. dvaju vektora

konjugirano (poteza)

$$\vec{x} \cdot \vec{y} = \sum_n x_n y_n^* = \sum_n x_n \bar{y}_n$$ jer komp. mogu biti i kompleksni brojevi

$$\vec{x} \cdot \vec{x} = \sum_n x_n x_n^* = \sum_n |x_n|^2 \geq 0$$ kvadrat iznosa ili „dužina" vektora

→ Koje transformacije ostavljaju dužinu vektora invarijantnom ?

$$A\vec{x}\cdot\vec{y} = \vec{x}\cdot A^{\dagger}\cdot\vec{y}$$

tj. $A\vec{x}\cdot\vec{y} = \vec{x}\cdot A^{*}\cdot\vec{y}$ gdje $A^{*} = (\bar{A})^{\perp}$ hermitski konjug. matrica

tj. $A^{\dagger} = (A^{*})^{\perp}$

$x_n' = (A\vec{x})_n = \sum_m a_{nm} x_m$

$$\sum_n \Big(\sum_m a_{nm} x_m\Big) y_n^{*} = \sum_m x_m \cdot \sum_n a_{nm} y_n^{*} = \sum_m x_m \cdot \sum_n (a_{nm}^{*}) y_n^{*} =$$

$$= \sum_m x_m \Big(\underbrace{\sum_n (a_{nm}^{*}\cdot y_n)}_{y_n' = \sum_n a_{nm}^{*} y_n \Rightarrow \vec{y}_n' = ((A^{*})^{\perp}\cdot\vec{y})_n}\Big)^{*} = \sum_m x_m \cdot \big((A^{*\perp}\cdot\vec{y})_n\big)^{*}$$

$$A\vec{x}\cdot A\vec{y} = \vec{x}\cdot A^{\dagger}\cdot(A\vec{y}) = \vec{x}\cdot A^{\dagger}\cdot A\cdot\vec{y}$$

zahtjev: $A\vec{x}\cdot A\vec{y} = \vec{x}\cdot\vec{y}$ specijalno $A\vec{x}\cdot A\vec{x} = \vec{x}\cdot\vec{x}$

$\Rightarrow$ $A^{\dagger}\cdot A = E$ tj. A unitarna matrica

$\Rightarrow$ $A = U$

$$U\vec{x}\cdot U\vec{x} = \vec{x}\cdot\vec{x}$$

→ unitarne transformacije ne mijenjaju dužine vektora i možemo ih tumačiti slično kao ortogonalne $AA^{\perp} = E$ transformacije.
To su vrtnje n-dim. prostora

→ Pri zakretu koordinata transformira se vektor u Hilbert-ovom prostoru po zakonu:

$$\vec{x}' = U\cdot\vec{x} \qquad x_n' = \sum_m u_{nm} x_m$$

$(\ ) = (\ )\cdot(\ )$

$$\vec{x}'^{*} = U^{*}\vec{x}^{*} \qquad x_n'^{*} = \sum_m u_{nm}^{*} x_m^{*}$$

tako se transformiraju kompleks. konjug. vrij. koordinata

$$U^{\dagger}\cdot U = E \Rightarrow U^{\dagger} = U^{-1} \Rightarrow U^{*} = (U^{-1})^{\perp}$$

$$\Rightarrow \vec{x}'^{*} = U^{-1\perp}\cdot\vec{x}^{*} \Rightarrow x_n'^{*} = \sum_m u_{mn}^{-1}\cdot x_m^{*}$$

$(\ ) = (\ )\cdot(\ )$

– u Hilbert-ovom prostoru možemo elem. matrica tumačiti kao elem. tenzora

transformacijski zakon tenzorskih elemenata izveli smo iz invarijantne konstrukcije tenz. računa

$$\vec{y} = A \cdot \vec{x} \qquad \left(\text{tenzorski: } \vec{y} \cdot \vec{x} = A \cdot \vec{x} \cdot \vec{x} = A \cdot E \quad ! \right)$$

$$(\,) = (\quad)(\,) \qquad (\,)(\,) = (\quad)(\|)(-)$$

tenzorski: $\vec{x} \cdot \vec{y} = [(x_n \cdot y_m^*)_{nm}]$ specijalno $\vec{x} \cdot \vec{x} = [(x_n \cdot x_m^*)_{nm}]$

$$(\,)(\quad)$$

$$\vec{x}' = U \cdot \vec{x} \qquad x_n' = \sum_m u_{nm} x_m$$

$$\vec{y}' = U \cdot \vec{y} \qquad y_n' = \sum_m u_{nm} y_m \Rightarrow y_n'^* = \sum_m u_{nm}^* y_m^* = \sum_m u_{mn}^{-1} \cdot y_m^*$$

tenzorski: $\vec{x}' \cdot \vec{y}' = [(x_n' \cdot y_m'^*)_{nm}] = [(\sum_k u_{nk} x_k \cdot \sum_l u_{lm}^{-1} y_l^*)_{nm}]$

$$x_n' \cdot y_m'^* = \sum_k \sum_l u_{nk} x_k \cdot y_l^* u_{lm}^{-1}$$

specijalno:

$$x_n' x_m'^* = \sum_k \sum_l u_{nk} x_k x_l^* u_{lm}^{-1}$$

elementi tenzora se transformiraju kao produkti komponenata vektora

– pri unitarnoj transformaciji Hilbert-ova prostora transformiraju se elem. matrice A prema zakonu:

$$\left.\begin{aligned} \vec{y} &= A \cdot \vec{x} \\ \vec{y}' &= U \cdot \vec{y} \\ \vec{x}' &= U \cdot \vec{x} \end{aligned}\right\} \Rightarrow \vec{y}' = U \cdot A \cdot \vec{x} = \underbrace{U A \cdot U^{-1}}_{A'} \vec{x}'$$

U^{-1} U^{-1}

$$\Rightarrow A' = U A U^{-1}$$

$$a_{nm}' = \sum_l (UA)_{nl} u_{lm}^{-1} = \sum_l \left(\sum_k u_{nk} a_{kl} \right) u_{lm}^{-1}$$

$$a_{nm}' = \sum_k \sum_l u_{nk} a_{kl} u_{lm}^{-1}$$

a to se podudara s izvedenim transf. pravilom za komponente tenzora

→ Klasični zakoni bili su invarijantni prema translaciji i vrtnji običnog prostora
Isto tako moraju i ovdje osnovni zakoni biti invarijantni prema „vrtnji" Hilbert-ova prostora.

→ Heisenberg-ova komutaciona pravila su invarijantna, ako od matrica p_0 & q_0 prijeđemo unitarnom transformacijom na nove matrice p & q

$$pq - qp = U p_0 U^{-1} \cdot U q_0 U^{-1} - U q_0 U^{-1} U p_0 U^{-1}$$

$$= U (p_0 q_0 - q_0 p_0) U^{-1}$$

ako $p_0 q_0 - q_0 p_0 = \frac{\hbar}{i} \cdot E \Rightarrow pq - qp = \frac{\hbar}{i} E$

→ općenito: Heisenberg-ova komutac. pravila su invarijantna prema transformacijama tipa

$$A' = TAT^{-1}$$ T - nemora biti unit. transf.

iz jbi. gibanja (Vanons U.h) → H dijag. matrica

- neka matrice p_0, q_0 zadovoljavaju Heisenberg-ova komutaciona pravila, ako uvrstimo matrice p_0, q_0 u Hamilt. fju. nekog atomnog sistema, općenito neće $H(p_0, q_0)$ biti dijagonalna matrica. Međutim, jednom unitarnom transformacijom p_0 & q_0 možemo postići, da Hamilt. fja. poprimi dijag. formu.
Problem je istovjetan s transformacijom tenzora na glavne osi.
Postoji uvijek jedan koordinatni sistem, u kojemu tenzor ima samo dijagonalne elemente. Određivanje diskretnih energija atomnog sistema svedeno je time na transformaciju matrice na glavne osi.

$$\left.\begin{array}{l} \vec{c} = A\vec{b} \\ \vec{c}' = U\vec{c} \\ \vec{b}' = U\vec{b} \end{array}\right\} \quad \vec{c}' = \underbrace{U A U^{-1}}_{A'} \cdot \vec{b}' \Rightarrow \underline{A' = U A U^{-1}}$$

$$A\vec{b} = (\alpha_{\alpha})\vec{b} \Rightarrow (A - \alpha^{-1}) \cdot \vec{b}_0 = 0$$

( )( )

→ Obzirom da M_x, M_y, M_z nisu istovremeno sve dijagonalne matrice, ali su u slučaju centralnih sila konstante gibanja tj. komutiraju s H

(*) ⇒ H degenerirana dijag. matrica*) (postoji isti elementi na dijagonali) degeneriranog atomnog sistema

Odaberimo M_z dijagonalnu: $M_z = \hbar L_z$

dalji račun opravdava pretp.

pretp.: dijagonalni elem. od L_z jednaki cijelim brojevima

$m = -l, \dots 0, \dots l$

redove i stupce matrica M_x, M_y, M_z numerirano po cijelom broju m

*) → naš kvantni sistem ima $2l+1$ različitih stanja jednake energije

→ koja čine jednu submatricu koja ima $(2l+1)$ redova ili stupaca, tj. njihov index ide $m = -l, \dots 0, \dots l$

$$(L_z)_{sub.} = \begin{pmatrix} \ddots & & \\ & m & \\ & & \ddots \end{pmatrix} \leftarrow m$$

to je polna submatrica od L_z istoenerg.

$$L_+ \cdot L_- - L_- \cdot L_+ = 2 L_z$$

$$L_+ = L_x + i L_y = [(\mu^+_{mn})_{mn}]$$

$$L_- = L_x - i L_y = [(\mu^-_{mn})_{mn}]$$

L_x, L_y, L_z hermitske matrice

$$\mu^+_{mn} = (\mu_x)_{mn} + i(\mu_y)_{mn}$$

$$\mu^-_{mn} = (\mu_x)_{mn} - i(\mu_y)_{mn}$$

$$\Rightarrow \mu^{*}_{mn} = (\mu_x)^*_{mn} + i^*(\mu_y)^*_{mn} = (\mu_x)_{mn} - i(\mu_y)_{mn} = \mu^-_{mn}$$

$$\Rightarrow \mu^{*\text{-Hermit.}}_{mn} = \mu^-_{mn}$$

$$2m = 2(L_z)_{mm} = \sum_n \mu_{mn}\underbrace{\mu^-_{nm}}_{\mu^*_{mn}} - \underbrace{\mu^-_{mn}}_{\mu^*_{nm}}\mu_{nm}$$

$$2m = \sum_n |\mu_{mn}|^2 - |\mu_{nm}|^2$$

Hermitske matrice čine aditivnu Abelovu grupu pa su i L_x & L_y Hermitske

→ tu jbu. možemo riješiti, da postavimo, da su od nule različiti samo elementi: $\mu_{m\,m-1} \neq 0$ ostali $= 0$

$$\mu_{m+1\,m} = \sqrt{l(l+1) - m(m+1)} = \sqrt{(l-m)(l+m+1)}$$

$$\mu_{m\,m-1} = \sqrt{l(l+1) - (m-1)m} = \sqrt{(l-m+1)(l+m)}$$

$$\Rightarrow \sum_n |\mu_{mn}|^2 - |\mu_{nm}|^2 = -(m-1)m + m(m+1) = +m(-m+1+m+1) = 2m$$

$$\Rightarrow m = -l, \dots 0, \dots l$$

$l = 0$ $\quad L_z = (0)$ $\quad L_+ = [\mu] = (0)$ $\quad |0\,0\rangle$

$l = 1$ $\quad L_z = \begin{pmatrix} -1 & & \\ & 0 & \\ & & +1 \end{pmatrix}$ $\quad L_+ = [\mu] = \begin{pmatrix} 0 & & \\ \sqrt{2} & 0 & \\ & \sqrt{2} & 0 \end{pmatrix}$ $\quad |1\,-1\rangle \quad |1\,0\rangle \quad |1\,1\rangle$

$l = 2$ $\quad L_z = \begin{pmatrix} -2 & & & & \\ & -1 & & & \\ & & 0 & & \\ & & & 1 & \\ & & & & 2 \end{pmatrix}$ $\quad L_+ = [\mu] = \begin{pmatrix} 0 & & & & \\ 2 & 0 & & & \\ & \sqrt{6} & 0 & & \\ & & \sqrt{6} & 0 & \\ & & & 2 & 0 \end{pmatrix}$ $\quad |2\,-2\rangle \quad |2\,-1\rangle \quad |2\,0\rangle \quad |2\,1\rangle \quad |2\,2\rangle$

(*) m2 (11) c)

$l=1 \qquad L_z = \begin{pmatrix} -1 & & 0 \\ & 0 & \\ 0 & & 1 \end{pmatrix}$

$$L_z\,|1\,m\rangle = m\,|1,m\rangle$$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}_{1,m} = \begin{pmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & m \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}_{1,m}$$

$$\begin{pmatrix} -1-m & 0 & 0 \\ 0 & -m & 0 \\ 0 & 0 & 1-m \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$(-1-m)\,x_1 + 0\cdot x_2 + 0\cdot x_3 = 0$$
$$0\cdot x_1 - m x_2 + 0\cdot x_3 = 0$$
$$0\cdot x_1 + 0\cdot x_2 + (1-m)\,x_3 = 0$$

$\langle 1,m|1\,m\rangle = 1$

$x_1^2 + x_2^2 + x_3^2 = 1$

netrivialno rješ.

$$\Rightarrow \begin{vmatrix} -1-m & 0 & 0 \\ 0 & -m & 0 \\ 0 & 0 & 1-m \end{vmatrix} = 0$$

$$(-1-m)(-m)(1-m) = 0 \quad \Rightarrow m_1 = -1,\ m_2 = 0,\ m = 1$$

$\underline{m_1 = -1} \Rightarrow x_2 = 0,\ x_3 = 0 \Rightarrow x_1 = \pm 1 \qquad |1,-1\rangle = \begin{pmatrix} \pm 1 \\ 0 \\ 0 \end{pmatrix}$

$m_2 = 0 \Rightarrow x_1 = 0,\ x_3 = 0 \Rightarrow x_2 = \pm 1 \qquad |1\,0\rangle = \begin{pmatrix} 0 \\ \pm 1 \\ 0 \end{pmatrix}$

$m_3 = 1 \Rightarrow x_1 = 0 \quad x_2 = 0 \quad x_3 = \pm 1 \qquad |1\,1\rangle = \begin{pmatrix} 0 \\ 0 \\ \pm 1 \end{pmatrix}$

(⊃ 11) $m = 2, \dots 2l$ zapravo $\underbrace{-l+1, \dots 0, l}_{2l}$

$$L_+ = \begin{array}{c} \\ m \rightarrow \end{array} \begin{pmatrix} 0 & 0 & 0 & 0 & & & 0 \\ & \ddots & \ddots & \ddots & & & \\ & & \mu_{m-1\,m-1} & 0 & & & \\ & & & \ddots & \ddots & & \\ & & & & \ddots & 0 & \\ 0 & & & & & \ddots & 0 \\ & & & & & & 0 \end{pmatrix}$$

$m-1$ $\quad$ m

tipa $(2l+1, 2l+1)$

$$\mu_{m\,m-1} = \sqrt{(l+m)(l-m+1)}$$

$$\mu^*_{mm} = \mu^-_{mm} \Rightarrow L_- = L_+^\dagger$$

$$L_- = \begin{array}{c} \\ m-1 \rightarrow \end{array} \begin{pmatrix} 0 & 0 & 0 & \cdots & & \\ & \ddots & \ddots & \ddots & & \\ & & 0 & \mu_{m-1\,m} & & \\ & & & \ddots & \ddots & \\ 0 & & & & \ddots & \ddots \end{pmatrix}$$

m

$$\Rightarrow \mu^-_{m-1\,m} = \mu^*_{m\,m-1} = \mu_{m\,m-1}$$

$$\dagger \cdot L_- = L_+^\dagger$$

$$|l\,m\rangle = \begin{array}{c} \\ 2l+1 \end{array} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \begin{array}{l} -l \\ -l+1 \\ \\ \leftarrow m \\ \\ l \end{array}$$

$$L_+ |l\,m\rangle = \begin{array}{c} -l \\ m \\ m+1 \rightarrow \end{array} \begin{pmatrix} 0 & 0 & 0 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \mu_{m-1\,m} & 0 & & \\ & & & \ddots & \ddots & \\ & & & & \ddots & 0 \\ & & & & \mu_{m+1\,m} & \\ & & & & & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \begin{array}{l} \\ \\ \\ \leftarrow m \\ \\ \\ \end{array} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \mu_{m+1\,m} \\ 0 \\ \vdots \end{pmatrix} \begin{array}{l} \\ \\ \\ \leftarrow m \\ \\ \\ \\ \end{array} = \mu_{m+1\,m} |l\,m+1\rangle$$

$$= \sqrt{(l-m)(l+m+1)}\, |l\,m+1\rangle$$

$$= 0 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \text{ za } m = l$$

$$L_- |l\,m\rangle = \begin{array}{c} m-1 \rightarrow \\ m \end{array} \begin{pmatrix} 0 & 0 & 0 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \mu^-_{m-1\,m} & 0 & & \\ & & & \ddots & \ddots & \\ & & & & \ddots & 0 \\ & & & & \mu^-_{m\,m+1} & \\ & & & & & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \begin{array}{l} \\ \\ \\ \leftarrow m \\ \\ \\ \end{array} = \begin{pmatrix} 0 \\ \mu^-_{m-1\,m} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{array}{l} -l \\ \leftarrow m-1 \\ \\ \\ l \end{array}$$

$$= \mu^-_{m-1\,m} |l\,m-1\rangle$$

$$= \mu_{m\,m-1} |l\,m-1\rangle$$

$$= \sqrt{(l+m)(l-m+1)}\, |l\,m-1\rangle$$

$$= 0 = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \text{ za } m = -l$$

(xx) iz (1)c) & zadatka 7.

$$L_z \underbrace{L_+^p |lm\rangle}_{L_z |lm\rangle = m|lm\rangle} = (m+p) \underbrace{L_+^p |lm\rangle}$$

dokazano za $p = 0, 1, 2, 3, \ldots$

za fiksirani $m = -l, \ldots 0, \ldots +l$

$L_+^p |lm\rangle$ je jedan od vlastitih vektora od L_z $|lm\rangle$ $m = -l, \ldots, l$

sa jednom od svojstvenih vrijednosti $-l, \ldots 0, \ldots l$

$$\Rightarrow L_+^p |lm\rangle \sim |l\, m+p\rangle$$

$$|l\, m+p\rangle \neq 0 = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \text{za} \quad -l \leq m+p \leq l \quad \Rightarrow$$

$$\left.\begin{array}{l} \Rightarrow -l-m \leq \underline{p \leq l-m} \quad \Rightarrow p_{max} = l-m \\ \& \quad p \geq 0 \\ \& \; -l \leq m \leq l \Rightarrow l \geq -m \geq -l \Rightarrow 0 \geq -l-m \geq -2l \end{array}\right\} \Rightarrow$$

$$\Rightarrow -l-m \leq \underline{0 \leq p \leq l-m} \leq 2l \Rightarrow p_{max} = l-m$$

$$\Rightarrow p = 0, 1, 2, \ldots (l-m)$$

- analogija: plan. model & ē oko jezgre

ē oko svoje osi - to možemo samo raditi na temelju analogija jer ē ne možemo proglasiti kuglicom, jer je to oblak naboja

→ spin elem. čestica: 1/2 u jedinicama $\hbar$

za elektron: (*)

$$\vec{M} = \vec{S} = \frac{\hbar}{2}\vec{\sigma}$$

Paulijeve matrice

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$M^2 = \hbar^2 l(l+1) E$

$$S^2 = \hbar^2 \cdot \frac{1}{2} \cdot \frac{3}{2} \qquad l = \frac{1}{2}$$

$$S^2 = \frac{\hbar^2}{4}(\sigma_x^2 + \sigma_y^2 + \sigma_z^2) = \frac{\hbar}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right]$$

$$= \frac{\hbar^2}{4} \cdot 3 \cdot E = \hbar^2 \cdot \frac{1}{2} \cdot \frac{3}{2}$$

što je M^2 za $l = \frac{1}{2}$ tj. spin je $\frac{1}{2}$

$l = \frac{1}{2} \Rightarrow m = \frac{1}{2}, -\frac{1}{2}$ na os kvantiz.

Supak 31.

(*) Taj moment projekcija $S_z = m \cdot \hbar$ $m = \frac{1}{2}, -\frac{1}{2}$ više ne možemo tumačiti gibanjem čestice oko nekе točke i nema veze s poč. definicijom momenta impulsa kao vektorskog produkta $\vec{M} = \vec{r} \times \vec{p}$, no on se može pripisati čestici kao njeno strukturno svojstvo

Experimenti:

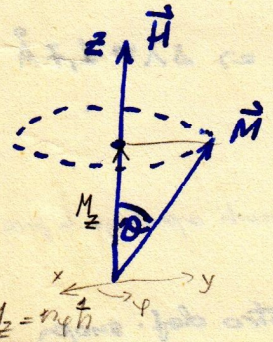
Zeeman-ov efekt (1896)

- normalni → 3 linije cijepanja ($s = 0$)
- anomalni → više linija → spin $s = \frac{1}{2}$ tj. njegov utjecaj

$\vec{M}$ magn. dipolni moment $\vec{\mu} = \frac{e}{2m_e c}\vec{M}$ Klas. relacija

elektroni u magn. polju $\vec{H}$

→ energija interakcije s $\vec{H}$



$p_\varphi = M_z = m_\varphi \hbar$

Supak II 28.

$M^2 = \hbar^2 l(l+1)$

$M = \hbar\sqrt{l(l+1)} \approx \hbar \cdot l$ za $l \gg$

tj. dobili smo Bohr-ovu pretp.

a $M_z = \hbar m$ $m = \pm l, \dots 0$

projekcije $\vec{M}$ na os z

- angularni moment $\vec{M}$ čini dodatno procesionogibanje tj. komponenta

$m = -l, \dots l$ harm. gibanje

$$M_{z_{mm}} = \hbar m \delta_{mm} \qquad m = \pm l, \dots 0$$

$M_z = p_\varphi = \vec{r} \times \vec{v} = mr^2\dot{\varphi}$

$$U_{pot} = -\vec{\mu} \cdot \vec{H} = -\frac{e \cdot M_z}{2m_e c} \cdot H$$

$$U_{pot} = -\frac{e\hbar}{2m_e c} \cdot mH \qquad m = \pm l, \dots 0$$

Bohr-ov magneton

$$\mu_B = \frac{|e|\hbar}{2m_e c} = 0{,}9273 \cdot 10^{-20} \ \frac{erg}{gauss}$$

el. j. em

energ. ē izvan $\vec{H}$

$$E' = E + U \qquad U = -\mu_B m H$$

energija ē u vanj. polju $\vec{H}$

$$\Delta U = -\mu_B H \cdot \Delta m$$

→ frekvencije koje može atomni sistem emitirati u magn. polju

$$\omega' = \frac{\Delta E'}{\hbar} = \frac{\Delta E}{\hbar} + \frac{\Delta U}{\hbar} = \omega + \Delta\omega$$

$$\Rightarrow \Delta\omega = \pm \frac{\mu_B \cdot H}{\hbar} \Delta m$$

$$= -\frac{|e|}{2m_e c} \cdot H = 2\pi \cdot \nu_L$$

- ne nalazi se $\hbar$ (kratiše se) → moglo se objasniti klasično tj. s Larmorovom frekvencijom ν_L

→ koje su moguće promjene Δm ?

na osnovu principa korespondencije za 1 gore ili dolje

$$\Delta m = 0, \pm 1 \Rightarrow \text{cijepanje na tri linije}$$

Mod. fizika 428.

njih je našao Zeeman 1896. ⇒ diskretnost u orijentacijama magnetskih momenata

→ neometano lin. titranje elektrona u smjeru $\vec{H}$ korespondira prijelazu $\Delta m = 0$, pri kojem se frekv. ne mijenja

→ oba klasična cirkularna titranja, pri kojima se frekvencija (cijepanja) mijenja za $\nu_L = -\frac{eH}{4\pi m_e c}$ korespondiraju prijelazima $\Delta m = \pm 1$

drugi prijelazi u kvantnoj teoriji nisu mogući, jer za njih nema klasičnog analogona

Klasično:

→ po Larmor. teoremu, elektr. sistemu u magn. polju pridolazi jednolika rotacija s frekvencijom ν_L već prema tome, da li se ē okreću oko magn. silnica u pozit. ili neg. smjeru, frekv. će se elektrona povećati ili umanjiti za ν_L

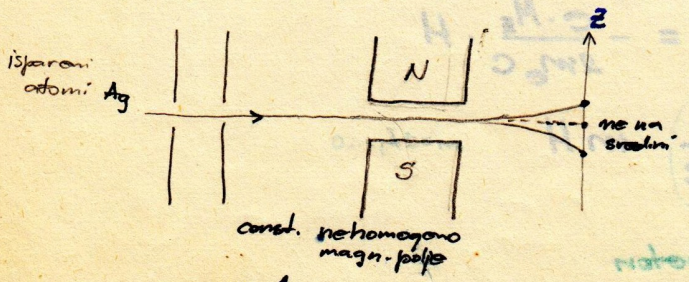
- oni ē koji titraju lin. u smjeru $\vec{H}$, neće uopće promijeniti ν

→ općenito ∀ titranje ē možemo rastaviti u ta tri tipična

$\Delta\omega$ se opaža samo u jačim poljima $H = 10^5$ Ga ⇒ $\Delta\lambda = 1{,}7$ Å

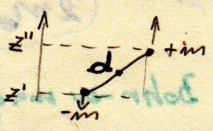
Stern - Gerlach (1922)

- doveo do hipoteze o spinu
- metod za mjerenje atomskih magneta i njihovih orijentacija u prostoru



Mjerenje pomaka ošto def. snopa na zastoru

∃ grad. polja u smjeru z-osi



$$H(z'') = H(z') + \frac{dH(z')}{dz}(z'' - z') + \dots$$

$$d\cos(d,z)$$

$$m H(z'') - m H(z') = \frac{dH}{dz} m d \cos(d,z) \Rightarrow F = \mu \frac{dH}{dz} \cos(d,z)$$

$$F = \mu \frac{dH}{dz} \cdot \cos(d,z)$$

- u const. homog. magn. polju atomski bi magneti bili samo zakrenuti oko svojeg središta

očekujemo:

$$U_{pot} = -\vec{\mu}\cdot\vec{H} = -\mu H \cos\vartheta$$

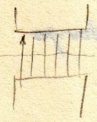
$$\vec{\mu} = \frac{e}{2m_e c}\cdot\vec{M}$$

$$\mu\cos\vartheta = \frac{e}{2m_e c}\cdot M_z$$

$$\vec{F} = -\nabla U_{pot} = \underbrace{\mu\cos\vartheta}_{\mu_B\cdot m = \frac{eM_z}{2m_e c}\cdot m}\nabla H \qquad \frac{dH}{dz} \neq 0$$

$\frac{dH}{dz}$ odred., μ - atomna konst.

→ varijabilna veličina je samo $\vartheta = \measuredangle(\vec{H},\vec{\mu})$, F odred. otklon od početnog smjera magnet.



$\vartheta = \frac{\pi}{2} \Rightarrow F = 0$ atom nesmetano

$\vartheta = 0 \Rightarrow F = +$

$\vartheta = \pi \Rightarrow F = -$ } najveći otklon.

sila: $-\mu\frac{dH}{dz}$ .... $\mu\frac{dH}{dz}$ kontinuirano

→ klas. teorija dozvoljava sve ϑ ⇒ raspršenje snopa Ag na kontinuum staza

očekujemo → pruga kojoj intenzitet opada prema krajevima

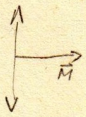
Maxwell. raspodjela

eksperiment: samo dva snopa (bez središnjeg)

$l = 0, 1, 2, \ldots \qquad m = -l, \ldots +l$

$l = 0 \qquad m = 0$

$l = 1 \qquad m = -1, 0, 1$



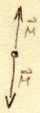
$m = 0 \Rightarrow \mu\cos\vartheta = \mu_B\cdot m = 0 \Rightarrow \vartheta = \frac{\pi}{2}$

neotklonjeni u njih nema

$l = 2$

$M_z = m\cdot\hbar$

⇒ uvođenje polucijelih



$l = \frac{1}{2} \qquad m = -\frac{1}{2}, +\frac{1}{2}$

$l = \frac{3}{2}$

Goudsmit - Uhlenbeck: momentu impulsa $\bar{e}$ oko jezgre pridodaje još vrtnja $\bar{e}$ oko svoje osi — analogija

$M_z = S_z = \pm\frac{\hbar}{2}$ ⇒ elektronu pripada magn. moment

$$\mu_e \neq \frac{e}{2m_e c}\cdot\frac{\hbar}{2} \qquad \text{već} \quad \mu_e = \mu_B = \frac{e}{2m_e c}\cdot\hbar$$

Visoke vrijedi klas. relacija između meh. mom. i magn. mom.

⇒ ukupni magn. moment atoma više vrede pada u isti smjer sa cjelokupnim meh. momentom

Schrödinger-ova valna jba.

Valovi materije:

Einstein: foton $p = \frac{h}{\lambda}$ $p = \hbar k$ $k = \frac{2\pi}{\lambda}$

$E = \hbar\omega$

de Broglie: (1924)

obrnuti zahvat - sve čestice možemo shvatiti i kao valove materije

→ gdje ∃ veza

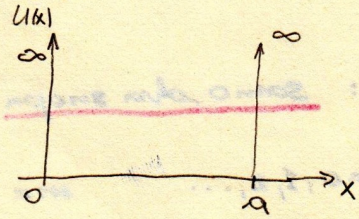
valna slika

stojni valovi

$a = n \cdot \frac{\lambda}{2}$

slično kao da čestu zatvorimo u pot. jamu

Korpuskularna slika



$\oint p\,dx = nh$ $\int_0^a p\,dx + \int_a^0 p\,dx$

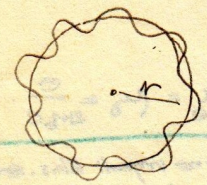
$2a\,p = nh$

$a = n\frac{h}{2p}$

ako ∃ analogija.

$\Rightarrow$ $\lambda = \frac{h}{p}$ isto kao i za fotone

→ Kretanje ē u kružnici. ako postoje stojni val



$2r\pi = n\lambda \Rightarrow r = \frac{n\lambda}{2\pi}$

$\vec{M} = \vec{r} \times \vec{p}$ $p_\varphi = n\hbar = r \cdot p \Rightarrow r = \frac{n\hbar}{p}$

$\frac{\lambda}{2\pi} = \frac{\hbar}{p}$

$\Rightarrow \lambda = \frac{h}{p}$

→ Bohr $\omega_{nm} = \frac{E_n - E_m}{\hbar}$

→ de Broglie ∀ čestici pripada $\omega = \frac{E}{\hbar}$ $\lambda = \frac{h}{p}$ $\Rightarrow p = \hbar k$

∀ čestici pridružujemo neki „oblak" koji nije ostro definiran

Ilustracije:

1) elektron u H-atomu

$$v \approx 10^8\,cm\,s^{-1} \qquad \lambda = \frac{h}{p} = \frac{h}{mv} \approx 6\cdot 10^{-8}\,cm$$

2) elektron u potencijalu V

$$E = |e|V \qquad p = \sqrt{2mE} = \sqrt{2m|e|V}$$

$$\Rightarrow \lambda = \frac{h}{\sqrt{2m|e|V}} = \sqrt{\frac{150}{V}}\ \text{Å}$$

– za makroskopske čestice $\lambda \to 0$ mala da ne primjećujemo

$$h \to 0 \Rightarrow \lambda \to 0$$

→ skepsa prema tim smjelim idejama

experimenti:

Davisson - Germer (1921)

analiza Ruth. pramjera – el. polje jezgre
el. polje el. oblaka

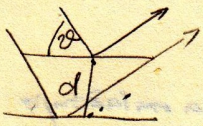
→ mjerenje angularne distribucije raspršenih zraka e^- na ploči nikla

- u valnoj slici: interferencija → max. i min. → pojava max. i min.
- objavljeno 1923.

Elsasser – max. i minim. mogu se objasniti de Broglie-ovom hipotezom

D.-G. (1927) ponovili exp.

→ ponašanje analogno Bragg-ovu exp.



$$n\lambda = 2d\sin\vartheta$$

ϑ – fiksni kut upada – mijenjamo λ pomoću V

⇒ promjena difrakcione slike max. & min. !

→ dat ćemo jbu. koja opisuje valove materije
- ne možemo je izvesti

relativistička čestica:

$\beta = \frac{v}{c}$

$$E = \frac{mc^2}{\sqrt{1-\beta^2}} \qquad p = \frac{mv}{\sqrt{1-\beta^2}}$$

$$\left(\frac{E}{c}\right)^2 = \frac{m^2c^2}{1-\beta^2} \qquad p^2 = \frac{m^2v^2}{1-\beta^2} \qquad \left(\frac{E}{c}\right)^2 - p^2 = \frac{m^2(c^2-v^2)}{1-\beta^2} = m^2c^2\frac{(1-\beta^2)}{1-\beta^2}$$

$$\left(\frac{E}{c}\right)^2 - p^2 = m^2c^2$$

energija pozitivna $\quad E = c\sqrt{p^2 + m_0^2c^2}$

specijalno:

el. magn. val → foton $\quad m=0 \quad \Rightarrow E = cp$

val materije: $\quad p = \frac{h}{\lambda} = \hbar k \qquad \left(\frac{\hbar\omega}{c}\right)^2 - \hbar^2k^2 = (mc)^2$

$$\Rightarrow \left(\frac{\omega}{c}\right)^2 - k^2 = \left(\frac{mc}{\hbar}\right)^2 \quad \overset{m=0}{\Rightarrow} \quad \frac{\omega}{c} = k \qquad (c = \nu\lambda)$$

1-Dim. ravni val

$$\psi(x,t) = Ae^{i(kx-\omega t)}$$

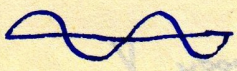
promatrajmo kako se u prostoru i vremenu kreću točke iste faze

$$kx - \omega t = const$$

$$k\,dx - \omega\,dt = 0$$

$$u = \frac{dx}{dt} = \frac{\omega}{k} = \nu\cdot\lambda \text{ fazna brzina} \qquad \frac{\omega}{k} = \frac{\omega}{\frac{p}{\hbar}} = \frac{\omega\hbar}{p}$$

(1) $A = const$



→ svugdje jednaka amplituda za nalaženje npr. e^-
- raznačen je po prostoru

→ za lokalizaciju čestice → superpozicija valova oblika $\psi(x,t) = A e^{i(kx-\omega t)}$

$$\psi(x,t) = \int_{k_0-\Delta k}^{k_0+\Delta k} A_1(k)\, e^{i(kx-\omega t)}\, dk$$

– suma kontinuiranog spektra valova između $[k_0-\Delta k,\ k_0+\Delta k]$

$$\sum_{j=-n}^{n} A(k_0+j\cdot\Delta k_1)\, e^{i[(k_0+j\cdot\Delta k_1)x-\omega(k_0+j\cdot\Delta k_1)\cdot t]}$$

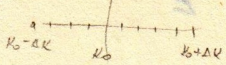
gdje $\Delta k = n\cdot\Delta k_1 \Rightarrow \Delta k_1 = \frac{\Delta k}{n}$

$n\to\infty \Rightarrow \Delta k_1 \to 0$ & $k_0+j\Delta k_1 \to k$

$$\xrightarrow{n\to\infty} \int_{k_0-\Delta k}^{k_0+\Delta k} A_1(k)\, e^{i[kx-\omega t]}\, dk$$

gdje $A(k_0+j\cdot\Delta k_1) = \underbrace{A_1(k_0+j\cdot\Delta k_1)}_{\text{gustoća ampl. po } k}\cdot\Delta k$

k_0 gustoća ampl. po k



napomena!!!

$A_1(k)$ gustoća amplitude val. fje. koja otpada na interval $(k, k+dk)$

pretp: gustoće amplitude se ne mijenjaju znatno sa k u intervalu $(k_0-\Delta k,\ k_0+\Delta k)$

tj. $A(k) \approx A(k_0)$

$$k = k_0 + (k-k_0)$$

$$\omega(k) = \omega[k_0+(k-k_0)] = \underbrace{\omega(k_0)}_{\omega_0} + (k-k_0)\left(\frac{d\omega}{dk}\right)_{k_0} + \dots$$

zanemarimo jer $\Delta k \ll$

$$e^{i(kx-\omega t)} = e^{i\left\{[k_0+(k-k_0)]x - [\omega_0+(k-k_0)\frac{d\omega}{dk}]t\right\}}$$

$$\frac{1}{i[x-\ ]}\, e^{i(k-k_0)[\ ]}\Big|_{k_0-\Delta k}^{k_0+\Delta k} = \frac{1}{i[\ ]}\left\{e^{i\Delta k[\ ]} - e^{-i\Delta k[\ ]}\right\} = \frac{1}{i[\ ]}\cdot 2i\sin\Delta k[\ ]$$

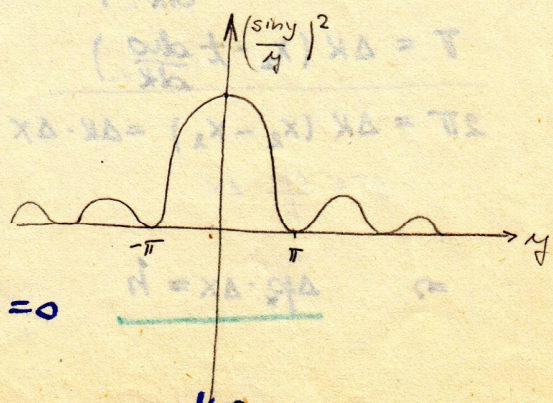
$$\psi(x,t) \approx A(k_0)\, e^{i(k_0x-\omega_0 t)} \cdot \int_{k_0-\Delta k}^{k_0+\Delta k} e^{i(k-k_0)\left(x-t\left(\frac{d\omega}{dk}\right)_{k_0}\right)}\, dk$$

$$= \underbrace{2A(k_0)\Delta k\, \frac{\sin\left[\Delta k\left(x-t\left(\frac{d\omega}{dk}\right)_{k_0}\right)\right]}{\Delta k\left[x-t\left(\frac{d\omega}{dk}\right)_{k_0}\right]}}_{\text{nova amplituda } B(k_0,\Delta k,x,t)}\, e^{i(k_0x-\omega_0 t)}$$

uvedemo: $y = \Delta k\left(x-t\left(\frac{d\omega}{dk}\right)_{k_0}\right) = y(k_0,\Delta k,x,t)$

$$\Rightarrow B \sim \frac{\sin y}{y}$$

→ intenzitet $\sim \frac{\sin^2 y}{y^2}$



→ max. za $y = \Delta k\left(x-t\left(\frac{d\omega}{dk}\right)_{k_0}\right) = 0$

$$x - t\left(\frac{d\omega}{dk}\right)_{k_0} = 0$$

$$\Rightarrow V = \frac{d\omega}{dk}$$ grupna brzina

veza grupne i fazne brzine $\left(\frac{\omega}{c}\right)^2 - k^2 = \left(\frac{mc}{\hbar}\right)^2$

$$\frac{2\omega d\omega}{c^2} - 2k\,dk = 0$$

$$V = \frac{d\omega}{dk} = \frac{c^2 k}{\omega}\frac{\hbar}{\hbar} = c^2 \cdot \frac{p}{E} = c^2 \cdot \frac{\frac{mv}{\sqrt{1-v_k^2}}}{\frac{mc^2}{\sqrt{1-v_k^2}}} = V$$ širenja čestice

!!! ovo nije

$$V = \frac{c^2}{\frac{\omega}{k}} = \frac{c^2}{u} \Rightarrow \underbrace{u}_{\text{fazna brzina}} = \frac{c^2}{\underbrace{V}_{\text{grupna brzina}}}$$

$V \leq c \Rightarrow u \geq c$ fazna brzina je matem. pojam., tj. brzina vala sa strogo određ. frekvencijom

no u prirodi nikada nedolaze titranja strogo određene frekvencije - pogledaj na 16

Sepek II 47.

→ ∀ je stvarno titranje zbroj jednostavnih ravnih valova različitih ν. Njihove frekv. mogu se usko gomilati oko jedne određene frekvencije, tako da imamo oštru spektralnu liniju, ali ustvari je to uvijek mnogo harmoničkih valova

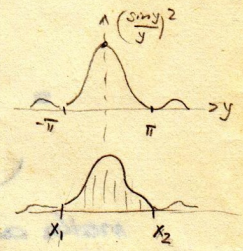
→ Relacije neodređenosti

Klas. fizika - poznavanje trajektorije $x(t)$

prip. impuls $p_x = m\frac{dx}{dt}$

Quant. fizika - dualnost → nemoguće odrediti p_x & x

$p = \frac{h}{\lambda}$ - veličina jednaka na ∀ mjestu



Izvod kvalitativnim razmatranjem:

valni paket između x_1 & x_2 u trenutku t

$\psi(x,t) = 2A(k_0)\cdot\Delta k \cdot \frac{\sin y}{y} e^{i(k_0 x - \omega_0 t)}$

$y = \Delta k\left(x - t\left(\frac{d\omega}{dk}\right)_{k_0}\right)$

$$\Rightarrow -\pi = \Delta k\left(x_1 - t\left(\frac{d\omega}{dk}\right)_{k_0}\right)$$

$$\pi = \Delta k\left(x_2 - t\left(\frac{d\omega}{dk}\right)_{k_0}\right)$$

$$2\pi = \Delta k\,(x_2 - x_1) = \Delta k \cdot \Delta x$$

$p = \hbar k \Rightarrow \Delta p = \hbar \cdot \Delta k$

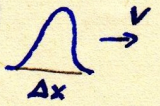
$$2\pi = \frac{\Delta p}{\hbar}\cdot\Delta x$$

$$\Rightarrow \Delta p_x \cdot \Delta x = h$$

energija - vrijeme

$$E = \frac{p^2}{2m} \qquad \Delta E = \frac{p \cdot \Delta p}{m}$$

valni paket prolazi kroz neku točku, a budući je širok Δx u vremenu Δt



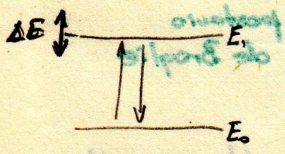
$$\Delta t = \frac{\Delta x}{v}$$

$$\Delta E \cdot \Delta t = \frac{p \cdot \Delta p}{m} \cdot \frac{\Delta x}{v} = \Delta x \cdot \Delta p$$

$$\Delta E \cdot \Delta t \approx h$$

Ilustracija:

čestica koja kratko vrijeme boravi u nekom kvantnom stanju $\rightarrow \Delta t$



$\Delta t = \tau$ - vrijeme života boravka u pobuđenom kvantnom stanju

tj. neodređeno vrijeme boravka u tom pobuđ. stanju koje je zbog prolaska valnog paketa širine Δx kroz tu točku (stanje)

$\nu = \frac{E_1 - E_0}{h}$ $\quad E_0$ - odred.

širina nepoznatog energetskog nivoa E_1 $\quad \Delta E_1 = \Delta E$

$\Delta \nu = \frac{\Delta E_1}{h} = \frac{\Delta E}{h}$

$$\Delta E \cdot \tau \approx h \Rightarrow \Delta \nu \cdot \tau = 1$$

$E = \hbar\omega = h\nu$

$\Rightarrow$ prirodna širina spektralne linije

$$\nu = \frac{c}{\lambda} \qquad \frac{1}{\tau} = \Delta\nu = \frac{c}{\lambda^2} \cdot \Delta\lambda \Rightarrow \Delta\lambda = \frac{\lambda^2}{c\tau} \quad *)$$

uzmimo:

$\tau = 10^{-8}\,s$

$\lambda = 6 \cdot 10^{-5}\,cm \Rightarrow \Delta\lambda \approx 10^{-11}\,cm$

Schrödinger-ova jba.

Iskonstruiramo dif. jbu. u skladu sa

$$\left(\frac{\omega}{c}\right)^2 - k^2 = \left(\frac{mc}{\hbar}\right)^2 \quad / \cdot \psi \qquad (*)$$

1-D im. $\quad \psi(x,t) = A e^{i(kx-\omega t)}$

$$\frac{\partial \psi}{\partial x} = ik\psi \qquad \frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi$$

$$\frac{\partial \psi}{\partial t} = -i\omega\psi \qquad \frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi$$

$$(*) \Rightarrow \quad -\frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} + \frac{\partial^2 \psi(x,t)}{\partial x^2} = \left(\frac{mc}{\hbar}\right)^2 \psi(x,t)$$

$$\psi(\vec{r},t) = A e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

$$-\frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} + \Delta\psi(\vec{r},t) = \left(\frac{mc}{\hbar}\right)^2 \psi(\vec{r},t)$$

postavio de Broglie

Svojstva i motivacija

1) Interferencija - suma rješenja je rješenje (linearnost)

2) Foton $m=0$ $\quad -\frac{1}{c^2}\ddot{\psi} + \Delta\psi = 0$ el. magn. val

iz Maxw. jbi $\Rightarrow \vec{\nabla}^2 \vec{E} - \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = 0$

općenito: $\vec{B} = \vec{\nabla}\times\vec{A}$

$$\vec{\nabla}^2 \vec{A} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = -\frac{\vec{j}}{\varepsilon_0 c^2}$$

$$\vec{\nabla}^2 \phi - \frac{1}{c^2}\frac{\partial^2 \phi}{\partial t^2} = -\frac{\varrho}{\varepsilon_0}$$

→ Promatramo monokromatske valove materije

$$\psi(\vec{r},t) = U(\vec{r}) e^{-i\omega t}$$

tj. pojedinačne valove fiksiranih ω

$$\ddot{\psi} = -\omega^2 U(\vec{r}) e^{-i\omega t} \qquad \Delta\psi = e^{-i\omega t}\Delta U(\vec{r})$$

$$-\frac{1}{c^2}(-\omega^2) U \cancel{e^{-i\omega t}} + \cancel{e^{-i\omega t}}\Delta U = \left(\frac{mc}{\hbar}\right)^2 \cancel{e^{-i\omega t}} \cdot U(\vec{r})$$

$$\Delta U(\vec{r}) + \underbrace{\left(\frac{\omega^2}{c^2} - \frac{m^2c^2}{\hbar^2}\right)}_{k^2} U(\vec{r}) = 0$$

$$k^2 = \frac{p^2}{\hbar^2}\frac{2m}{2m} = \frac{2m}{\hbar^2}\cdot E$$ kin. energija

$$\Rightarrow \quad \Delta U(\vec{r}) + \frac{2m}{\hbar^2} E \cdot U(\vec{r}) = 0$$

vrijedi za slobodnu česticu

jer E je kin. energija, a mi je ni smo označili sa E_k, već sa E što znači ukupna energija

Schrödinger (1926) - korak dalje

$$E = \frac{p^2}{2m} + U = E_k + U$$

$$\Delta u_{(\vec r)} + \frac{2m}{\hbar^2}\overbrace{(E-U)}^{E_k} u_{(\vec r)} = 0$$

amplitudna Schröd. jba.

jer $\psi(\vec r, t) = u(\vec r)\, e^{-i\omega t}$

→ formalan izvod:

Klas. fizika — Hamiltonova fja. neovisna o vrem. tj. konst. gibanja - neovisi expl. o t - stacionaran klas. problem.

$$H = \frac{p^2}{2m} + U = E$$

općenito $H \equiv H(x_1, \dots z_n, p_{x_1}, \dots p_{z_n}) = E$

i Schröd. jba. izražava $H = E$

Komutacijska pravila za kvantne veličine $[\hat u, \hat v] = i\hbar\{u, v\}_{PB}$

$\Rightarrow$ $[\hat x_j, \hat x_k] = 0$ $[\hat y_j, \hat y_k] = 0$ $[\hat p_{x_j}, \hat p_{x_k}] = 0$ $[\hat p_{y_j}, \hat p_{y_k}] = 0$ $[\hat x_j, \hat p_{x_k}] = i\hbar\delta_{jk}$ $[\hat x_j, \hat p_{y_k}] = 0$ j-ta i k-ta čestica

zadovoljena ako $\hat x_j, \hat y_j, \hat z_j$ uzmamo kao veličine koje podliježu obionoj algebri, dok $\hat p_{x_k}, \hat p_{y_k}, \hat p_{z_k}$ kao dif. operatore

$$\hat p_{x_k} = -i\hbar\frac{\partial}{\partial x_k} \quad \hat p_{y_k} = -i\hbar\frac{\partial}{\partial y_k} \quad \hat p_{z_k} = -i\hbar\frac{\partial}{\partial z_k}$$

→ tada za proizv. fju. $f(x_1, \dots z_n)$ vrijedi

$$[\hat x_j, \hat x_k] f = 0 \quad [\hat p_{x_j}, \hat p_{x_k}] f = 0 \quad [\hat x_j, \hat p_{x_k}] f = i\hbar\delta_{jk} f$$

y $=0$, z $=0$; p_y $=0$, p_z $=0$; p_{y_k} $=0$, p_{z_k} $=0$

→ za kvantni analogon klasičnog problema izvršimo zamjenu klas. veličina s kvantnima u H

$$\hat H \equiv H\left(x_1, \dots z_n, -i\hbar\frac{\partial}{\partial x_1}, \dots -i\hbar\frac{\partial}{\partial z_n}\right) = E$$

operatorom $\hat H = E$ djelujemo na valnu fju $\psi(x_1, \dots z_n, t)$ tj. na njenu amplitudu $u(x_1, \dots z_n)$

Kvantne veliči:

$$\vec p \to \frac{\hbar}{i}\vec\nabla = \frac{\hbar}{i}\sum \vec i \frac{\partial}{\partial x} \qquad p_x \to \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$p^2 \to \left(\frac{\hbar}{i}\vec\nabla\right)^2 = -\hbar^2\vec\nabla^2 = -\hbar^2\Delta$$

$$H(\vec p, \vec r) \to \hat H\left(\frac{\hbar}{i}\vec\nabla, \vec r\right) = -\frac{\hbar^2}{2m}\Delta + U \quad \text{- operator}$$

$$\underset{\text{operator}}{\hat H}\, u(\vec r)\, e^{-i\omega t} = E\, \overbrace{u(\vec r)\, e^{-i\omega t}}^{\psi(\vec r, t)\ \text{valna fja}} \Rightarrow -\frac{\hbar^2}{2m}\Delta u + U u = E u$$

$$\Rightarrow \Delta u(\vec r) + \frac{2m}{\hbar^2}(E-U)\, u(\vec r) = 0$$

Klas. veliči. p — Kvantni operator

- amplitudna Schröd. jba $\quad H u = E u \quad / \cdot e^{-i\omega t}$

$H\psi = E \cdot \psi$

de Broglie - u čestičnom slučaju:

$$\omega = \frac{E}{\hbar} \qquad \lambda = \frac{h}{p}$$

$$\psi(\vec{r},t) = u(\vec{r}) \cdot e^{-i\omega t} = u(\vec{r}) \cdot e^{-\frac{i}{\hbar}E \cdot t}$$

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E \cdot \psi$$

$$H\psi = E \cdot \psi = E \left(-\frac{\hbar}{iE}\right) \frac{\partial \psi}{\partial t}$$

$$\hat{H}\, \psi(\vec{r},t) = -\frac{\hbar}{i} \frac{\partial \psi(\vec{r},t)}{\partial t}$$

vremenski ovisna Schröd. jba.

dok H fja. položaja ne ovisi expl. o t

$\hat{H} = -\frac{\hbar^2}{2m}\Delta + U$

- nerelativistička!

- linearna homogena parcij. dif. jba II reda

→ Sistem s različitim energetskim nivoima

$$\psi_n = U_n(\vec{r})\, e^{-\frac{i}{\hbar}E_n t}$$

npr. elektron na E_n je opisan valom $\omega_n = \frac{E_n}{\hbar}$ $\quad \omega_{nn'} = \omega_n - \omega_{n'} = \frac{E_n - E_{n'}}{\hbar}$

$$H\psi_n = -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi_n \quad / \cdot c_n \sum_n$$

$H = E_n$ djel. na ψ_n

iz linearnosti jbe.

lin. operatori → homomorfizmi

$f(a \times b) = f(a) \times f(b)$

$$H \sum_n c_n \psi_n = -\frac{\hbar}{i}\frac{\partial}{\partial t} \sum_n c_n \psi_n$$

→ opće rješenje:

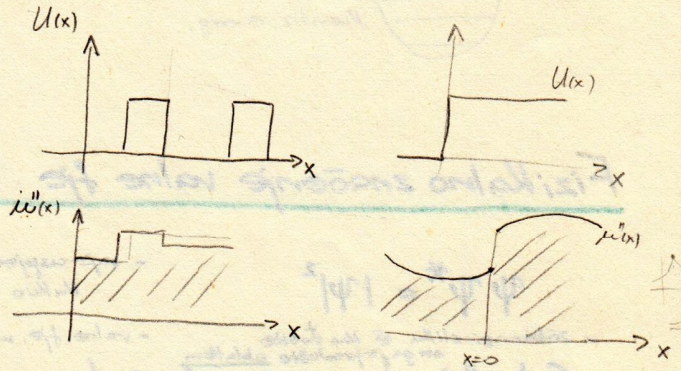
$$\psi(\vec{r},t) = \sum_n c_n \psi_n(\vec{r},t) = \sum_n c_n U_n(\vec{r})\, e^{-\frac{i}{\hbar}E_n t}$$

Sama Schröd. jba. ne daje kvantizaciju

→ zahtjevi regularnosti ⇒ energ. diskretnost

zahtjevi regularnosti

1-D im. $\quad u'' + \frac{2m}{\hbar^2}(E-U)u = 0$



(i) **Kontinuiranost** valne fje
- neprekinutost

na mjestu potencijalnog skoka, valna fja. i njena 1. derivacija moraju biti kontinuirane (nepr.)

$$u' = \int u''dx \qquad u = \int u'dx$$

u', a pogotovo u su nepr. fje. jer površina što je omeđuje x & $u''(x)$ kontinuirano raste, iako sama fja. čini skok. no površina upravo geom. znači integral fje. u''

(ii) **Konačnost** valne fje. posvuda

(iii) **jednoznačnost** valne fje.

iz zahtjeva kontinuiranosti 1. deriv. valne fje $\Rightarrow$

potencijalna energija smije imati samo takav prekid

$U(x) \to \infty$ proturječi (iii) pr iz jbe. $\Rightarrow u'' \to \infty \Rightarrow u(x) \to \infty$

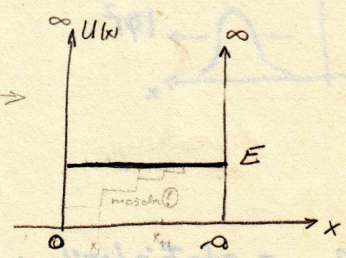
!!! pravdi: stože

$\overset{(*)}{\Rightarrow} u \to 0$ jedini sposb. da ne proturječi

kao zahtjev

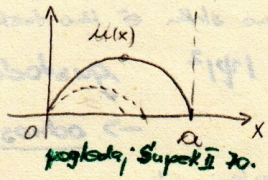
$u''(x_n) = 0 \quad u \neq 0 \Rightarrow E_n = U(x_n)$ diskretna vrij. energije na dok. mjestima x_n

(*) u protivnom kad bi $u \neq 0 \Rightarrow$ iz jbe. $u'' \to \infty$
$\Rightarrow u' \to \infty \Rightarrow u \to \infty$ a to se protivi (ii)



Ilustracija:

Pitanje: može li se energija kontinuirano mijenjati
→ mijenjala bi se zakrivljenost (u'') po predznaku
valna fja. bi pala na nulu prije točke a
$\xrightarrow{?}$ odr. - diskretnost energije (*)



pogledaj Šupek II 70.

$U(0) = U(a) = \infty \Rightarrow u(0) = u(a) = 0$

za $0 < x < a \quad U(x) = 0$

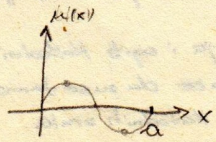
$\Rightarrow u'' + \frac{2m}{\hbar^2}Eu = 0$

$\Rightarrow u = A\cos\frac{\sqrt{2mE}}{\hbar}x + B\sin\frac{\sqrt{2mE}}{\hbar}x$

$u(0) = 0 \Rightarrow A = 0$

$u(a) = 0 \Rightarrow \frac{\sqrt{2mE}}{\hbar}a = n\cdot\pi$

$\Rightarrow E = n^2 \cdot \frac{\hbar^2}{8ma^2}$



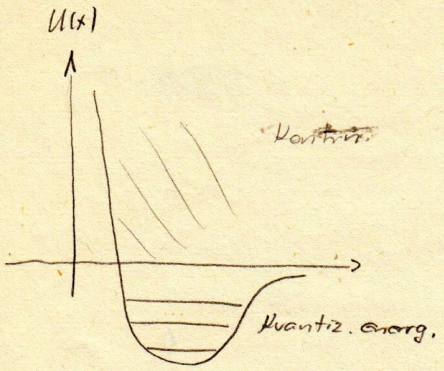
(*) valna teorija, bez ikakvih apriornih pretp., daje diskretan spektar energija

→ originalno !!!

napomena:
ako bi se $U(x)$ kontinuirano mijenjala tada bi za a $\lim_{x\to a-0} U(x)$ bio ∞, dok ovako je const. kad diskretnih vrijednosti

$\Rightarrow$ za $\lim_{x\to a-0}$ je $u''(x)$ tend. $u = 0$

$u(x) = A\sin kx + B\cos kx$
$u(0) = 0 \quad u(a) = 0$
$ka = n\pi$
$\Rightarrow u_n(x) = A\sin\frac{n\pi}{a}x$



Fizikalno značenje valne fje. $\psi(\vec{r},t)$

$$\psi\psi^* = |\psi|^2$$

- nije uspjelo valnim fjama materije pripisati neposredno fizičko značenje kakvo npr. imaju el. polja u valnim jdbama elektrodin.
- valne fje. materije ostaju u današnjoj teoriji matem. konstrukcije

- zamišljao sliku ē kao čestice ili gaj. prostornog oblakom

Schröd. je pretp. da je to u vezi s gustoćom naboja koji nosi ē

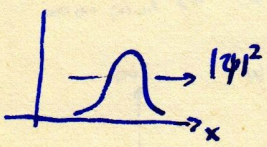
$$\rho = e|\psi|^2$$

integral po gustoći

$$e = \int \rho \underbrace{d\tau}_{dV} = \int e|\psi|^2 d\tau \Rightarrow \int |\psi|^2 d\tau = 1$$

neodrživost:

1) $|\psi|^2$ - velika prostorna protegnutost
- elektron se raspline

2) 

Supek II 58.

val materije (ē) bacimo na potencijalni bedem → val se na njemu djelom. reflektira, a djelomično se širi u poč. smjeru

→ valne fje. ∃ i s jedne i s druge strane

paradox: ē se reflektirao i odjurio dalje

!!!

Born - statistička interpret.

- zadržao sliku ē kao točkastog naboja

$\rho = |\psi|^2$ gustoća vjerojatnosti da ē nađemo negdje u prostoru

→ odnos vjerojatnosti transmisije u odnosu na refleksiju

- time valovi materije gube osjetljivo značenje, koje su im pripisali de Broglie i Schrödinger, i preostaju samo „valovi vjerojatnosti"

- interferencija i difr. katodnih zraka (Tebye - Scherrer) → tamna i svetla mjesta ne znače da susedamo ē poništili ili pojačali, već kako su često na ta mjesta pali ē katodnih zraka

- Born-ovo stat. tumačenje valova materije suočilo se ipak s teškoćama, kad prijeđemo u područje relativističke kvantne teorije, tako da još danas ne možemo tvrditi, da smo potpuno spoznali, što su pravo valovi materije znače. Ova nerazjašnjenost ne smeta nas ipak, ali na osnovu valnih fja. proračunamo mnoštvo svojstava atoma, a dobiveni rezultati trajno su postali teorije, bez obzira kakva će biti sudbina fizičkih shvaćanja o valnim fjama.

- val materije opisan sa $\psi(\vec{r},t)$

vjerojatnost nalaženja u djelu prostora $d\tau \rightarrow |\psi|^2 d\tau$

- po cijelom prostoru $\int |\psi|^2 d\tau = 1$ $\qquad \rho = |\psi|^2 = \psi \cdot \psi^*$

$\rightarrow$ $\forall$ gustoća povezana je s gustoćom struje

gibanja naboja, ili mase očitaju se kao struje

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \vec{j} = 0 \,/ e \qquad \rho_e = e \cdot \rho = e \cdot |\psi|^2$$

$$\frac{\partial \rho_e}{\partial t} + \operatorname{div} \vec{j}_e = 0 \qquad \vec{j}_e = e \cdot \vec{j}$$

jba. kontinuiteta, koja izražava neuništivost naboja

$$\frac{\partial}{\partial t} \rho = \dot{\psi} \psi^* + \dot{\psi}^* \psi \qquad H\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t}$$

$$\dot{\psi} = -\frac{i}{\hbar} H \psi$$

$$\dot{\psi}^* = \frac{i}{\hbar} H \psi^*$$

$$\hat{H} = -\frac{\hbar^2}{2m} \Delta + U$$

realan operator

$\Rightarrow \underline{H^* = \hat{H}}$

$$\frac{\partial}{\partial t} \rho = \frac{i}{\hbar} \left(\psi \cdot H \cdot \psi^* - \psi^* \cdot H \psi \right)$$

$$\hat{H} = \frac{1}{2m} \left(\frac{\hbar}{i} \right)^2 \Delta + U$$

$$\frac{1}{2m} \left(\frac{\hbar}{i} \right)^2 \left[\psi \Delta \psi^* - \psi^* \Delta \psi \right] + \cancel{\psi \cdot U \psi^* - \psi^* U \psi}$$

nije operator, već oblik

$$= \frac{1}{2mi} \hbar \left(\psi \Delta \psi^* - \psi^* \Delta \psi \right)$$

$$\underset{\text{div}}{\vec{\nabla} \cdot} \left(\psi \underset{\text{grad}}{\vec{\nabla} \psi^*} - \psi^* \underset{\text{grad}}{\vec{\nabla} \psi} \right) = \underset{\text{div}}{\vec{\nabla}} \left(\psi \underset{\text{grad}}{\vec{\nabla} \psi^*} \right) - \underset{\text{div}}{\vec{\nabla}} \left(\psi^* \underset{\text{grad}}{\vec{\nabla} \psi} \right) = \cancel{\underset{\text{grad}}{\vec{\nabla} \psi^*} \cdot \underset{\text{grad}}{\vec{\nabla} \psi}} + \psi \underset{\text{div grad}}{\vec{\nabla} (\vec{\nabla} \psi^*)}$$

$$- \cancel{\vec{\nabla} \psi \cdot \vec{\nabla} \psi^*} - \psi^* \underset{\text{div grad}}{\vec{\nabla} (\vec{\nabla} \psi)} = \psi \Delta \psi^* - \psi^* \Delta \psi$$

$$= -\frac{i\hbar}{2m} \vec{\nabla} \cdot \left(\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi \right) \quad (*)$$

$$\Rightarrow \underline{\vec{j} = \frac{i\hbar}{2m} \left(\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi \right)}$$

Zadatak: primjenimo na ravni val $\psi(\vec{r},t) = A e^{i(\vec{k} \cdot \vec{r} - \omega t)}$

pokazati $\vec{j} = \vec{v} \cdot \rho \qquad \vec{v} = \frac{\hbar \vec{k}}{m} \qquad \rho = |\psi|^2 = |A|^2$

pogledaj Supek II 59.

$\int |\psi|^2 d\tau = 1 \Rightarrow \quad \rho = |\psi|^2$ ne $\rho_e = e \cdot \rho$

$$\frac{\partial}{\partial t} \int_V \rho \, d\tau = 0 \quad \Rightarrow \quad \int \frac{\partial \rho}{\partial t} d\tau = 0$$

→ izvedimo zadano iz Schröd. jbe.

$$(*) \Rightarrow \quad \frac{\hbar}{2mi} \int_{div} \vec{\nabla} \cdot (\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi) \, d\tau = 0$$

→ Gauss-ov tm. $\int_V \operatorname{div} \vec{a} \, dV = \iint_P \vec{a} \cdot d\vec{F}$

$$\Rightarrow \quad \int_V (\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi) \, d\vec{f} = 0$$

? vjerojatno

→ promatramo (val. fje) rješenja koja iščezavaju na rubu naše površine koja čini Volumen V

dolje kao uputa

vrem. promj. Schröd. jba.

$$H\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t}$$

općenito $\psi(\vec{r}, t) = u(\vec{r}, t) e^{-i\omega t}$

→ za H koji ne ovisi explicito o t

za $\frac{\partial u}{\partial t} = 0$ separacija $\psi(\vec{r}, t) = u(\vec{r}) \cdot \varphi(t)$

$$\Rightarrow \quad \varphi H u = -\frac{\hbar}{i} u \frac{d\varphi}{dt} \quad / : u\varphi$$

oper. → $$\frac{\hat{H} u(\vec{r})}{u(\vec{r})} = -\frac{\hbar}{i} \frac{d\varphi(t)}{dt} \cdot \frac{1}{\varphi(t)} = \text{const.} = E$$

prost. deriv. vrem. deriv.

$\hat{H} = E$

$\hat{H} u(\vec{r}) = E u(\vec{r})$

$\frac{\hat{H} u}{u} = E$

(i) $\hat{H} u = E \cdot u$

(ii) $\frac{d\varphi}{dt} = -\frac{i}{\hbar} E \varphi \quad \Rightarrow \quad \varphi = C e^{-\frac{i}{\hbar} E \cdot t}$

$$\psi(\vec{r}, t) = \underbrace{u(\vec{r})}_{\text{sadrži } i\, C} e^{-\frac{i}{\hbar} E \cdot t}$$ - rješ. za sistem u stac. stanju energ. E

za niz stac. stanja

$$\psi(\vec{r}, t) = \sum_n C_n u_n(\vec{r}) e^{-\frac{i}{\hbar} E_n t}$$

Primjena Schröd. jbe. na:

1-D.m. amplitudnu jbu.

$$\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}(E-U)u = 0$$

1) $U=0$ -gibanje slob. čestice

$$u'' + k^2 u = 0 \qquad k^2 = \frac{2m}{\hbar^2}E = \frac{p^2}{\hbar^2} \qquad k = \frac{p}{\hbar}$$

$$u = Ae^{ikx} + Be^{-ikx}$$

$$\psi(x,t) = u(x)\cdot e^{-\frac{i}{\hbar}Et}$$

$$\psi(x,t) = \underbrace{Ae^{i(kx-\frac{E}{\hbar}t)}}_{(a)} + \underbrace{Be^{-i(kx+\frac{E}{\hbar}t)}}_{(b)}$$

(a) → val koji da bi sačuvali istu fazu $(kx-\frac{E}{\hbar}t)$ s porastom t ide u $+x$ smjeru

(b) → val u suprotnom smjeru

$$\left(\frac{\omega}{c}\right)^2 - k^2 = \left(\frac{mc}{\hbar}\right)^2$$

$E_n = \hbar\omega_n$

→ ←

Iz uvjeta $e^{ikx} = e^{ik(x+\lambda)} \Rightarrow e^{ik\lambda} = 1 \qquad k_n\lambda_n = 2\pi\cdot n$ (1 puda)

$$\Rightarrow u_n(x) = Ae^{ik_nx} + Be^{-ik_nx}$$

$$\lambda = \frac{2\pi}{k} = \frac{2\pi}{\frac{p}{\hbar}} = \frac{h}{p}$$ de Broglie-ova relacija

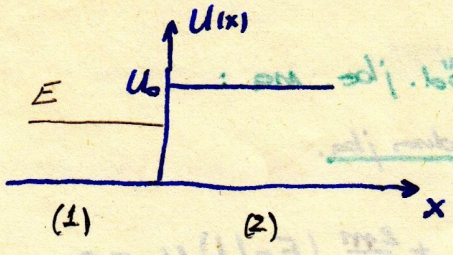
$$e^{-i\frac{E}{\hbar}t} = e^{-i\frac{E}{\hbar}(t+\tau)} \Rightarrow \frac{E_n}{\hbar}\cdot\tau_n = 2\pi\cdot n \qquad E_n = 2\pi\cdot\hbar\cdot\frac{1}{\tau_n}$$

$$\Rightarrow E_n = h\nu_n$$ de Broglie

dakle, Schröd. jba. za 1 česticu izbacuje de Broglie-ove relacije

2) (dodatak uz V1.-)

$$U = \begin{cases} 0 & x \le 0 \\ U_0 & x > 0 \end{cases}$$



a) val koji dolazi s energijom $E < U_0$ na potencijalni bedem

pretpostavka - energija nije kvantizirana

(moguće lijevo od potenc. bedema)

Schröd. jbu ćemo rješavati u dva područja

područje (1) $\quad u'' + k^2 u = 0 \qquad k^2 = \frac{2m}{\hbar^2} E$

(2) $\quad u'' - l^2 u = 0 \qquad l^2 = \frac{2m}{\hbar^2}(U_0 - E)$

$$u_{(1)} = \underset{\text{upadni val}}{A e^{ikx}} + B e^{-ikx}$$

$$u_{(2)} = C e^{-lx} + D e^{lx}$$

B ← reflekt. val iz pr. 1)

C → val koji je prošao u pot. bedem

$\psi_{(t)c} = C e^{-lx - i\frac{E}{\hbar}t} =$

→ uvjeti regularnosti

1° Konačnost

$u\ (2) \qquad u \not\to \infty$ za $x \to \infty$ (ne smijemo dopustiti)

$\Rightarrow D = 0 \qquad \Rightarrow \psi_2(x,t) = C e^{+lx - i\frac{E}{\hbar}t}$

napomena: za $x \to -\infty$ e^{-ikx} je ograničen $\hbar$. $|e^{-ikx}| = 1$ tako da ne mora biti $B = 0$

2° Kontinuiran prijelaz tj. čak „glatak" prijelaz

$u_1(0) = u_2(0) \quad \Rightarrow \quad A + B = C$

$u_1'(0) = u_2'(0) \quad \Rightarrow \quad ik(A - B) = -lC$

$A\left(1 + \frac{ik}{l}\right) + B\left(1 - \frac{ik}{l}\right) = 0$

$B = \frac{\frac{ik}{l} + 1}{\frac{ik}{l} - 1} A$

⇒ možemo proizv. odabrati ampl. upadnog vala A

⇒ odredeni B & C

$$B = A\,\frac{k - il}{k + il} \quad \Rightarrow \quad |B|^2 = |A|^2 \quad (*)$$

$$C = A\,\frac{2k}{k + il}$$

valu $\xrightarrow{\text{pridružujemo}}$ gustoću struje

$\rho_e = e\cdot\rho = e|\psi|^2$ $\quad \frac{\partial\rho}{\partial t} + \operatorname{div}\vec{j} = 0$

$\vec{j}_e = e\cdot\vec{j}$

$$\vec{j} = \frac{i\hbar}{2m}\left(\psi\cdot\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi\right)$$

1-Dim. $\quad \psi(x,t) = u(x)\cdot e^{-\frac{i}{\hbar}Et}$

$\psi^*(x,t) = u^*(x)\cdot e^{\frac{i}{\hbar}Et}$ $\qquad \vec{\nabla} = \vec{i}\frac{d}{dx} \qquad \vec{j} = j\cdot\vec{i}$

$$\Rightarrow \quad j = \frac{i\hbar}{2m}\left(u\frac{d}{dx}u^* - u^*\frac{d}{dx}u\right)$$

→ upadni val $\quad u_u = Ae^{ikx}$

$$j_u = \frac{i\hbar}{2m}\left(-ik|A|^2 - ik|A|^2\right) = \frac{\hbar k}{m}|A|^2$$

→ reflektirani val $\quad u_r = Be^{-ikx}$ $\quad$ ← u suprotnom smjeru

$u_r^* = B^*\cdot e^{ikx}$

$$j_r = \frac{i\hbar}{2m}\left(ik\cdot|B|^2 + ik|B^2|\right) = -\frac{\hbar k}{m}|B|^2$$

$$|j_r| = \frac{\hbar k}{2m}|B|^2 \overset{(*)}{=} \frac{\hbar k}{2m}|A|^2$$

$v = \frac{p}{m} = \frac{\hbar k}{m}$

$\rho = |\psi|^2 = |A|^2$

$\Rightarrow |j_r| = j_u = \frac{\hbar k}{m}|A|^2$

$j = \rho\cdot v$

→ lomljeni val $\quad u_l = Ce^{-lx}$ $\quad$ - realna fja $(\ ) = 0$

$u_l^* = C^*e^{-lx}$

$$j_l = \frac{i\hbar}{2m}\left(-l|C|^2 + l|C|^2\right) = 0$$

$\rho = |\psi|^2$

→ ne ∃ vjerojatnost da lomljeni val uđe u pot. barijeru (zbog $E < U_0$)

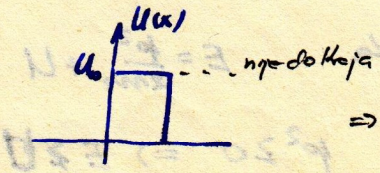
(*) $\Rightarrow |j_r| = j_u$

Koef. refleksije $\quad R = \frac{|j_r|}{j_u} = 1$

Koef. transmisije $\quad P = \frac{j_l}{j_u} = 0$

→ ali dakle, valna fja ∃ u (2)

- važno za slučaj



⇒ u tom slučaju očekujemo $P \neq 0$ kroz takav pot. barijeru

b) slučaj $E > U_0$

u prijelazu iba $\underline{l \to -il'}$ taj

$$u_{(2)} = C e^{ilx} + \underbrace{D e^{-ilx}}_{\text{odbacujemo iz vizualnog razloga}}$$

$il' = -l$

$\underline{l = -il'}$

$A + B = C$

$iK(A-B) = (il')C$ odgovara prijelazu $-l$

naime to riješ dobijemo ako

(2) $u'' + l^2 u = 0$ gdje $l^2 = \frac{2m}{\hbar^2}(E - U_0)$

- dao bi val od desna na lijevo - ne možemo poveza ti s fiz. pretpostavkom!

tada:

$$B = A\frac{K-l}{K+l}$$

$$C = A\frac{2K}{K+l}$$

$u_1(0) = u_2(0) \Rightarrow A + B = C$

$u_1'(0) = u_2'(0) \Rightarrow \cancel{i}K(A-B) = \cancel{i}l \cdot C$

$2A = \left(1 + \frac{l}{K}\right)C$

$B = A\frac{K-l}{K+l}$

$u_l = C e^{ilx}$

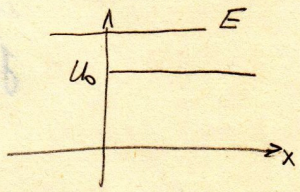
$$j_u = \frac{\hbar K}{m}|A|^2 \qquad |j_r| = \frac{\hbar K}{m}|B|^2 \qquad j_l = \frac{\hbar l}{m}|C|^2$$

$$|j_r| + j_l = \frac{\hbar K}{m}|A|^2\frac{(K-l)^2}{(K+l)^2} + \frac{\hbar l}{m}\cdot|A|^2\frac{4K^2}{(K+l)^2} =$$

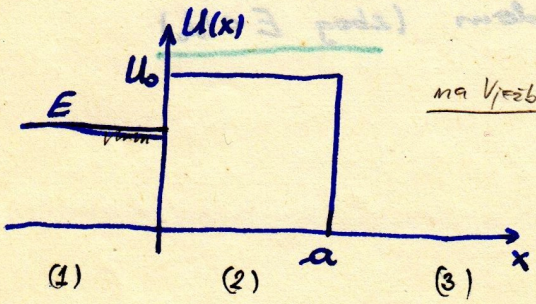
$$= \frac{\hbar K}{m}|A|^2 \cdot \frac{(K-l)^2 + 4Kl}{(K+l)^2} = j_u$$

$$R + P = \frac{|j_r|}{j_u} + \frac{j_l}{j_u} = 1$$

∃ samo vjerojatnost za reflex. i transmisiju ali nije 100% sigurno da dođe prod.



3)



na Vježbama

Pokazuje se da se val materije može reflektirati, ali i prod. kroz barijeru!

Klas. fizika $\quad E = \frac{p^2}{2m} + U$

zahtjev: čestica se giba samo dano gdje $|p| \geq 0 \Rightarrow p^2 \geq 0$ (*)

$p^2 \geq 0 \Rightarrow E \geq U$

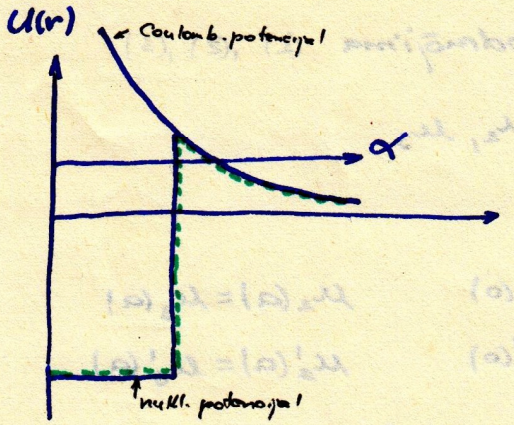
Kvantna fizika - ne ∃ relacija oblika (*) jer ne ∃ aps. definiran p.

$\Delta p \cdot \Delta x \approx h$

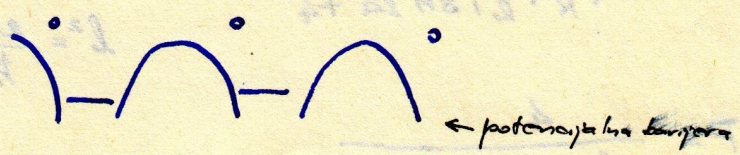
i ∃ tunel efekt - vezan u fizici

Tunel efekt :

α-raspad



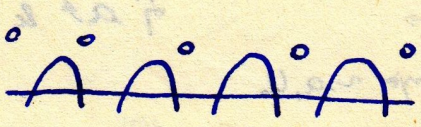
Kemijska veza H_2^+



tunel efekt elektrona → veza

vodljivost metala

∃ vjerojatnost prijelaza elektrona u područje susjednog atoma (nadbal)?
→ struja



→ pogledaj bolje te primjere tunel efekta !!!

→ rješenja po područjima (1), (2), (3)

u_1, u_2, u_3

i povezivanje:

$u_1(0) = u_2(0)$ $\qquad$ $u_2(a) = u_3(a)$

$u_1'(0) = u_2'(0)$ $\qquad$ $u_2'(a) = u_3'(a)$

& vježba 11. - pripadne gustoće struje

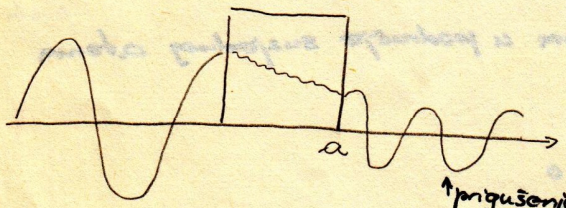
$$\Rightarrow \quad R = \frac{\left(\frac{l}{k} + \frac{k}{l}\right) sh^2 la}{\left(\frac{l}{k} + \frac{k}{l}\right)^2 sh^2 la + 4}$$

$$k^2 = \frac{2m}{\hbar^2} E$$

$$l^2 = \frac{2m}{\hbar^2} (U_0 - E) \qquad U_0 > E$$

$$P = \frac{4}{\left(\frac{l}{k} + \frac{k}{l}\right)^2 sh^2 la + 4}$$

$$R + P = 1$$



↑prigušenje ~ a, U_0

$P \to 0$ za veliko la

tj. $a\uparrow$ & $l\uparrow$ $(U_0\uparrow)$ $\Rightarrow P\downarrow$

$$sh\, la = \frac{e^{la} - e^{-la}}{2} = \frac{1}{2}\sum_{n=0}^{\infty} \frac{(la)^n}{n!} - \frac{(-la)^n}{n!} = \frac{1}{2}\left\{ \sum_{k=0}^{\infty} 2\frac{(la)^{2k+1}}{(2k+1)!} \right\} = \sum_{k=0}^{\infty} \frac{(la)^{2k+1}}{(2k+1)!} = la + \frac{(la)^3}{3!} + \frac{(la)^5}{5!} + \dots$$

→ Procjenimo uz $l \approx k$ (*) $\Rightarrow P \approx \frac{4}{4\, sh^2 la + 4} = \frac{1}{sh^2 la + 1} \gtrsim \frac{1}{2}$ za $sh^2 la \lesssim 1$

$\Rightarrow la \lesssim 1$

$k = \frac{2\pi}{\lambda}$, $\quad la \lesssim 1 \overset{(*)}{\Rightarrow} \frac{2\pi}{\lambda} \cdot a \lesssim 1 \qquad 2\pi a \lesssim \lambda$

Za prolaz kroz potenc. barijeru $\lambda \gtrsim a$

logično - iz očekivanih razlučivost se postiže kod valnih kopnenih λ

$sh\, al = \frac{e^{al} - e^{-al}}{2}$

Supek II 68:

ako je bedem dosta širok tj. $la \gg 1$

$$\Rightarrow P \approx \frac{16 E (U_0 - E)}{U_0^2} e^{-\frac{2a}{\hbar}\sqrt{2m(U_0 - E)}}$$

dokazati (**)

$$\Rightarrow P \approx \frac{4}{\left(\frac{l}{k} + \frac{k}{l}\right)^2 \cdot \frac{1}{4} e^{2al} + 4} = \frac{16}{16 + \left(\frac{l}{k} + \frac{k}{l}\right)^2 e^{2al}}$$

$$\approx \frac{16}{\left(\frac{l}{k} + \frac{k}{l}\right)^2} e^{-2al} = \frac{16}{\frac{l^2}{k^2} + \frac{k^2}{l^2} + 2} \cdot e^{-2al}$$

$$\frac{l^2}{k^2} + \frac{k^2}{l^2} = \frac{U_0 - E}{E} + \frac{E}{U_0 - E} = \frac{U_0^2 - 2U_0E + E^2 + E^2}{E(U_0 - E)}$$

$$\frac{l^2}{k^2} + \frac{k^2}{l^2} + 2 = \frac{U_0^2 - 2U_0E + 2E^2 + 2EU_0 - 2E^2}{E(U_0 - E)}$$

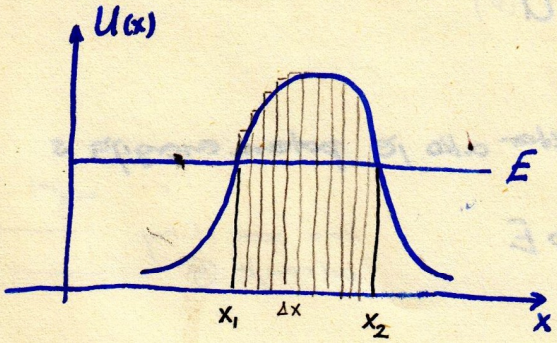
ukom slučaj koef. transmisije vrlo brzo opada sa širinom barijere a, masom čestice m i relativnom visinom barijere $U_0 - E$

ovisnost o masi

$$l = \frac{1}{\hbar}\sqrt{2m(U_0-E)}$$

→ **Opći slučaj**: za $la \gg 1$ pot. barijera dosta široka

vjerojatnost da čestica prođe kroz potencijalnu barijeru



za $U_0 > E$ & $la \gg 1$ Quasi Klas. limes tj. $l \gg 1$

$$P \approx \frac{16E(U_0-E)}{U_0^2}\, e^{-\frac{2a}{\hbar}\sqrt{2m(U_0-E)}}$$

ali ne $l \to \infty$ kao za $\hbar \to 0$

procjenjujemo po područjima !

1° $E > U$ izvod. $\Rightarrow P = 1$ za $a = \frac{n}{2}\lambda$

inače u najgorem slučaju za $a = (2n+1)\frac{\lambda}{4}$ (Vježbe 12.)

$$T = P = \frac{4\mathcal{K}^2 K^2}{(\mathcal{K}^2+K^2)^2} \quad \text{gdje} \quad \mathcal{K} = \frac{1}{\hbar}\sqrt{2m(E-U_0)}$$

→ za slike za $E>U$ tj. $x<x_1$, $x>x_2$ $U(x)$ naglo pada, tj. aproksimiramo $U(x)=0$!

$\Rightarrow \mathcal{K} = K \Rightarrow P = 1$

- ako i nije $P=1$, ali nikad nije P blizu nule, pa to u odnosu na dominantan faktor (**) ništa neznači

2° vjerojatnost prolaza kroz podan pravokutnik

$$P_1 \sim e^{-2\frac{\Delta x}{\hbar}\sqrt{2m(U_1-E)}}$$

$$\vdots$$

$$P_n \sim e^{-2\frac{\Delta x}{\hbar}\sqrt{2m(U_n-E)}}$$

$$\vdots$$

napomena !!!

- zanemarujemo faktor $\frac{16E(U_0-E)}{U_0^2}$ ($U(x)$) prema dominantnim faktorom (**)
- u Quasi Klas. limesu $l \gg 1$ tako da još možemo smatrati: $l \cdot \Delta x \gg 1$

$\Delta x \to 0$ apsurdno ! (*)

vjerojatnost prolaza kroz sve pravokutnike

$$P = \underbrace{1 \cdot 1 \cdots 1}_{\text{približno}} \cdot P_1 \cdot P_2 \cdots = e^{-\sum_n 2\frac{\Delta x}{\hbar}\sqrt{2m(U_n-E)}}$$

$E > U(x)$

prijelazom na i integral (*)

$$P = e^{-\int_{x_1}^{x_2} \frac{2}{\hbar}\sqrt{2m(U(x)-E)}\,dx}$$

za $la \gg 1$ $\quad l = \frac{1}{\hbar}\sqrt{2m(U_0-E)}$

Quasi Klas. limes

– približna formula

Opća svojstva jednodim. gibanja (Landau-Lifšic 58)

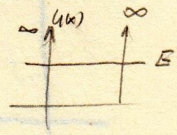
$\hat{H}\,u(\vec{r}) = E\,u(\vec{r})$ $\qquad \hat{H} = -\frac{\hbar^2}{2m}\Delta + U(\vec{r})$

*) amplid. Schröd

- diskretni spektar ako je potenc. energija s obje strane

$$U > E$$

Kao spec. slučaj od ranije (☆)



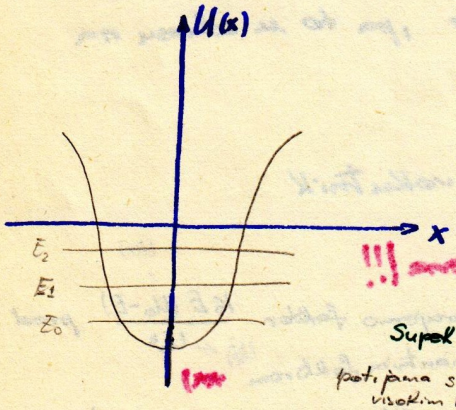
- valna fja. označava kvantna stanja

I degeneracija $\qquad u_1, u_2, \ldots$ (razlicite valne fje ali) iste energije E

$$\omega_{12} = \frac{E^{(1)} - E^{(2)}}{\hbar} = 0$$

- prijelazi povezani s frekv. koja iščezava

II Slučaj gdje nema degeneracije



→ ako na rubovima $U(R) = \infty$ tada nema degeneracije

$$u''(x) + \frac{2m}{\hbar^2}(E - U(x))\,u(x) = 0$$

pretp. $u(R) \neq 0 \Rightarrow u''(R) = \infty \Rightarrow u'(R) = \infty \Rightarrow u(R) = \infty$

no to nesmijemo dozvoliti: da val materije na rubovima postaje ∞ velik

!!! $\Rightarrow$ val. fja. iščezava na rubu $u(R) = 0$

Supak II t.

$\Rightarrow$ energija je kvantizirana

pošto imamo s ∞ visokim rubovima

rješavamo *)

$$u''(x) + k^2 u(x) = 0 \qquad k^2 = \frac{2m}{\hbar^2}(E - U(x))$$

pretp. dva rješenja za isti E →

$$u_1'' + k^2 u_1 = 0 \qquad u_1(R) = 0$$
$$u_2'' + k^2 u_2 = 0 \qquad u_2(R) = 0$$

} uvjeti regularnosti zbog zahtjeva konačnosti

$$\Rightarrow \frac{u_1''}{u_2''} = \frac{u_1}{u_2} \Rightarrow u_1'' u_2 - u_2'' u_1 = 0$$

$$\frac{d}{dx}\left(u_1'(x)\,u_2(x) - u_2'(x)\,u_1(x)\right) = 0$$

Sveučil II 12. (x) u2 (24)

$\hat{H} = \frac{\hbar^2}{2m}\Delta + U(x)$

$\hat{H}u(x) = E\,u(x) \Rightarrow$

$\Rightarrow$ $u(x)$ vlastita (vektor) fja. za dif. operator $\hat{H}$ i vlastitom vrijednosti E

$$(\hat{H} - E)\,u(x) = 0$$

$$\left(\frac{\hbar^2}{2m}\Delta + U(x)\right)u(x) = E\cdot u(x)$$

$$\left(\Delta + \frac{2m}{\hbar^2}U(x)\right)u(x) = \frac{2m}{\hbar^2}E\;u(x)$$

$u(x)$ vlast. fja. za dif. operator $\left(\Delta + \frac{2m}{\hbar^2}U(x)\right)$ i vlastit. vrijednosti $\frac{2m}{\hbar^2}E$

ako $U(-x) = U(x)$ & $\Delta = \frac{d^2}{dx^2}$ $\Rightarrow$ vlastite fje moraju biti sim. ili asim. na $x \to -x$

dokaz: neka $u_n(x)$ neko rješ. Schröd. jbe.
u jbi. se ne promijeni ništa ako $x \to -x$
što znači da $u_n(-x)$ mora biti rješ. za isti energetski term.

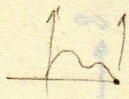
ostala rješenja su sim. i asim. kombinacija:

sim. $u(x) = u_n(x) + u_n(-x)$ asim. $u(x) = u_n(x) - u_n(-x)$

napomena: za $U(R) = \infty$ $u^{as}(-x) = u_n(-x) - u_n(x) = -u^{as}(x)$

$\rightarrow$ u jednodim. slučaju pripada jednom energetskom termu $E_n = E$ samo jedna vlastita fja. $u(x)$ $\Rightarrow$ jedno od gornjih rješ. mora iščezavati to znači da je već $u_n(-x) = u_n(x)$ ili $-u_n(x)$

$$\Rightarrow \quad u_1'(x)\,u_2(x) - u_2'(x)\,u_1(x) = C$$



uvjeti regularnosti: Konačnost $\Rightarrow$ $u_1(R) = u_2(R) = 0$

Kontinuiranost $\Rightarrow$ C isti za $\forall x$

$$\Rightarrow C = 0 \quad \rightarrow \quad \frac{u_1'(x)}{u_1(x)} = \frac{u_2'(x)}{u_2(x)} \quad \int dx \quad \Rightarrow \ln u_1(x) = \ln \bar{C}_1 + \ln u_2(x)$$

$$\Rightarrow \quad \underline{u_2(x) = C_1\, u_1(x)} \quad *)$$

- samo jedno lin. nezav. rješenje za $U(R) = \infty$ (rubni) tj. $\Leftrightarrow$ (suprotno) energija je kvantizirana

→ Specijalni slučajevi

Kad nema degeneracije

a) simetrična pot. energija $\quad U(x) = U(-x) \quad *)$

Schröd. $\rightarrow$

$$\overbrace{\left\{ \frac{d^2}{dx^2} + \frac{2m}{\hbar^2}\left[E - U(x)\right] \right\}}^{(*)} u_1(x) = 0 \qquad u_1(x) \text{ za } x > 0$$

$x \to -x$

$\frac{d}{dx} \to -\frac{d}{dx}$

$\frac{d^2}{dx^2} = \frac{d}{dx}\left(\frac{d}{dx}\right) \to -\frac{d}{dx}\left(-\frac{d}{dx}\right) = \frac{d^2}{dx^2}$

$$\longrightarrow \left\{ \frac{d^2}{dx^2} + \frac{2m}{\hbar^2}\left[E - U(x)\right] \right\} \overbrace{u(-x)}^{u_2(x)} = 0 \qquad u_2(x) \text{ za } x < 0$$

(možemo primijeniti, jer za $x>0$ & $x<0$ operator je nepromijenjen tj. i sama dif. jba., a pretp. dva različ. rješenja $u_1(x)$ & $u_2(x)$ za ta dva posebna područja

$$\Rightarrow \quad u(-x) = C\,u(x) \quad *)$$

$x \to -x$

$$u(x) = C\,u(-x) = C^2 u(x) \quad \Rightarrow \quad C^2 = 1 \quad \Rightarrow \quad C = \pm 1$$

jedina mogućnost za rješenje:

pogledaj papir (*) $\qquad \underline{u(-x) = \pm u(x)}$ (*) - rješenje se odlikuje paritetom + ili − tj. kad zrcaljenja $x \to -x$

općenito, ne gledajući *)

a)' → diferencijalni operator (x) je realan tj.

$$\{\quad\}^{*} = \{\quad\}$$

-konjugirano

$$\Rightarrow \{\quad\} u^{*} = 0 \quad \Big\} \Rightarrow u^{*}(x) = C\,u(x) \quad \Rightarrow u(x) = C^{*} u^{*}(x) = C^{*} \cdot C\, u(x)$$

$\{\quad\} u \to u_2(x)$; $u^{*} \to u_2(x)$; $u^{*}(x) \to u_2(x)$

$$u(x) = |C|^2 u(x) \quad \Rightarrow |C|^2 = 1$$

$$\Rightarrow \underline{C = e^{i\varphi}} \quad \text{opć. neodređen} \quad \Rightarrow u^{*}(x) = e^{i\varphi} u(x)$$

Koristili smo *)

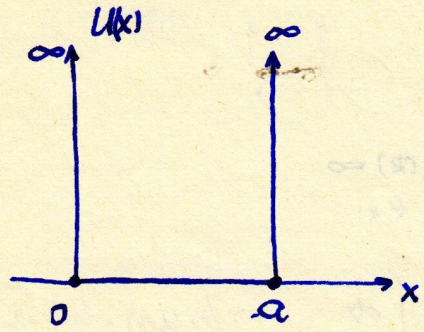
$$\Rightarrow \quad \underline{u(x) = e^{i\varphi} u^{*}(x)}$$

$\Rightarrow$ za kvantiz. energiju → realna valn fja.

u smislu da C nemora biti realno, a ona već kuta je adekvatno odrediti φ - obično $=0$

tj. nije $\psi(x) + i\,\psi(x) = u(x)$

b)



- u jednom dijelu prostora nema sile, a na rubu djeluje jaka sila koja ne dozvoljava prolaz

$$\vec{F} = -\vec{\nabla} U$$

$$U(x) = \begin{cases} \infty \\ 0 & 0 \le x \le a \\ \infty \end{cases}$$

→ pokazati ćemo da su u tom (*) području moguće samo odred. energije

$$\frac{d^2 u}{dx^2} + \frac{2m}{\hbar^2}(E-U)u = 0$$

uvjet regularnosti na val. fju.

$$U(R)=0 \Rightarrow_{(*)} \begin{cases} u(0)=0 \\ u(a)=0 \end{cases}$$

$$u'' + k^2 u = 0 \qquad k^2 = \frac{2m}{\hbar^2}E$$

$$u = A\sin kx + B\cos kx$$

$$u(0) = B \overset{(*)}{\Rightarrow} B = 0$$

nepotrebno $n=-1,-2,\ldots$ jer (*) → izmj. const.

$$u(a) = A\sin ka \overset{(*)}{\Rightarrow} ka = n\pi \qquad n = \overset{0}{\cancel{1}}, 2, 3, \ldots$$

općenito - kvantizacija slijedi iz uvjeta na valnu fju. - Schpolski 70.

$$k^2 = \frac{n^2\pi^2}{a^2} = \frac{2m}{\hbar^2}E \quad (*)$$

$$\Rightarrow \underset{\text{ne } (n-1)}{E_n} = \frac{\hbar^2\pi^2}{2ma^2}\cdot n^2$$

bolje: $E_{n-1} = \frac{\hbar^2\pi^2}{2ma^2} n^2$ jer $(n-1)$ daje broj čvorova valne fje

$$u_n(x) = \underline{A}\sin\frac{n\pi}{a}x$$

↓ treba odrediti, može biti i kompleksan

$$\psi(x,t) = u(x)\cdot e^{-\frac{i}{\hbar}Et} \qquad \psi^*(x,t) = u^*(x)\, e^{\frac{i}{\hbar}Et}$$

$$\int |\psi|^2 d\tau = 1 \qquad \int \psi\cdot\psi^* d\tau = \int u(x)\, u^*(x)\, d\tau = 1$$

→ opć. iz uvjeta : $\int_{-\infty}^{\infty} |u_n(x)|^2 dx = 1$

$$\int_0^a u_n^2(x)\, dx = 1 \qquad A^2 \int_0^a \sin^2 \frac{n\pi}{a} x\, dx = 1 \qquad \int_0^a \sin^2 \frac{n\pi}{a} x\, dx = \left(\frac{1}{2}x - \frac{1}{4\cdot\frac{n\pi}{a}} \sin \frac{2n\pi}{a} x\right)\Big|_0^a = \frac{a}{2}$$

realna, ali sadrži $|A|^2$

$$\Rightarrow |A|^2 = \frac{2}{a} \qquad \Rightarrow A = \sqrt{\frac{2}{a}}\, \underbrace{e^{i\varphi}}_{\text{odabiramo } = 1}$$

$$A = \sqrt{\frac{2}{a}}$$

valne fje. su ortogonalne -

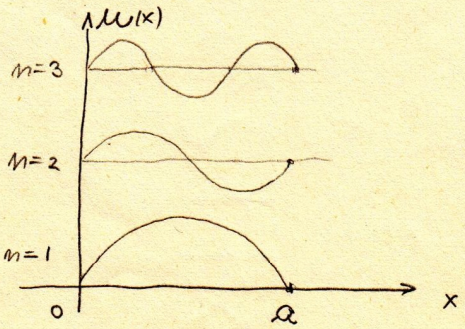
$$A\cdot A^* \int_0^a \sin \frac{n\pi}{a} x \cdot \sin \frac{m\pi}{a} x\, dx = 0 \qquad n \neq m$$

→ općenito za 1-Dim. problem

$$\int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx = \delta_{nm}$$

može se opć. pokazati

→ val. fja. pobuđenja :

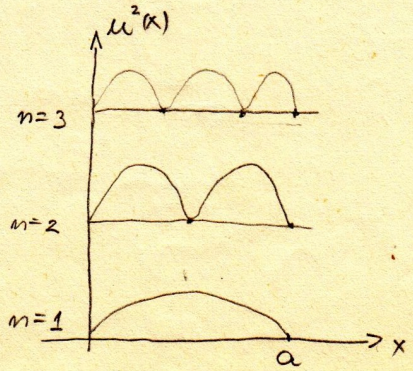


(n-1) broj čvorišta valne fje.

→ gustoća vjerojatnosti :

$$\rho = |\psi|^2 = \psi\cdot\psi^* = u\cdot u^* = u^2$$

realna



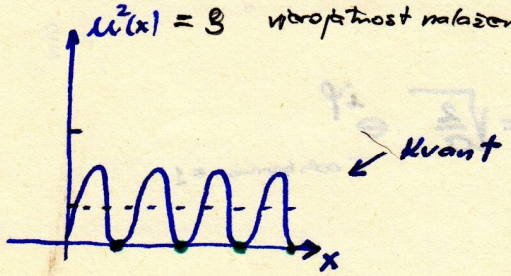
Klas. fizika: $U=0 \Rightarrow v=\frac{dx}{dt}=C$

$dW \sim dt=\frac{dx}{v}$ → u jednako velikim dif. elementima čestica boravi jednako dugo

vjerojatnost

tj. $\rho \sim \frac{1}{v}$ gustoća vjerojatnosti

Q. M.

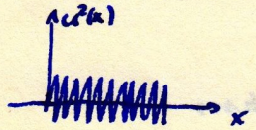


→ neki dif. elementi $\rho=0$ su zabranjeni

tj. vrijeme čestice provedeno u njima dif. elem. $=0$

za $t \sim \rho$

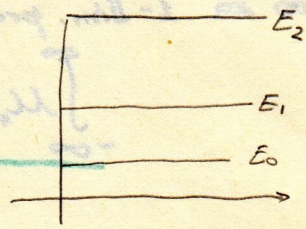
→ za visoke kvantne brojeve n



klas. ↓ usrednjeno

energija: $E_{n-1}=\frac{\hbar^2\pi^2}{2ma^2}n^2$ $n=1,2,\ldots$

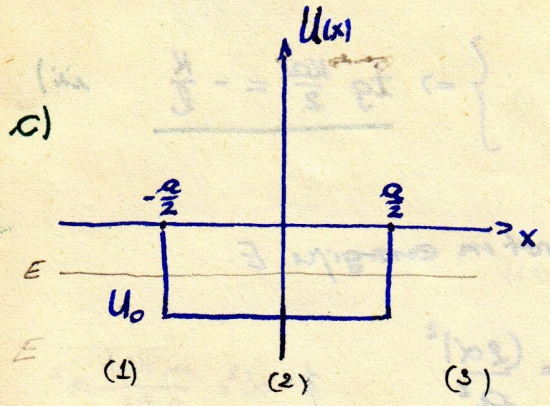
$(n+1)^2-n^2=2n+1$



∞ mnogo nivoa

za $U=0$ razmak raste sa n

c)



$$U(-x) = U(x)$$

papir (*) na 28 jer dano korišteno *) tj. da je $U(R)=\infty$

$$\Rightarrow \quad \underline{u(-x) = \pm u(x)} \quad *)$$

$$\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}(E-U)u = 0$$

za $\underline{E<0}$ & $|E|<|U_0|$ $E=-|E|$ $\quad U_0<0$

(1) $\frac{d^2u}{dx^2} - l^2 u = 0 \qquad l^2 = \frac{2m}{\hbar^2}|E|$

$+\frac{2m}{\hbar^2}(-|E|-U_0)$

(2) $u'' + k^2 u = 0 \qquad k^2 = \frac{2m}{\hbar^2}(\overset{>0}{-U_0}-|E|) > 0$ za $-U_0 > |E|$ tj. $|U_0|>|E|$

(3) $u'' - l^2 u = 0$

$\Rightarrow$ (1) $u = B_1 e^{-lx} + B e^{lx}$

(2) $u = A_1 \sin kx + A_2 \cos kx$

(3) $u = C_1 e^{-lx} + C_2 e^{lx}$

uvjeti regularnosti:

1° konačnost rješ. val. fje.

(1) $x \to -\infty \Rightarrow B_1 = 0$

(3) $x \to +\infty \Rightarrow C_2 = 0$

*) $\Rightarrow$ rješ. sim. ili asim. $u(x)$ iz čitavog područja $\quad u(x) = \begin{cases} Be^{lx} & x<-\frac{a}{2} \\ A_1 \sin kx + A_2 \cos kx & -\frac{a}{2}<x<\frac{a}{2} \\ C_1 e^{-lx} & x>\frac{a}{2} \end{cases}$

tj. dvije grupe rješ. po (1) (2) & (3) ili dva rješ. $u(x)$

$\Rightarrow B = C_1$ za sim.

$B = -C_1$ za asim.

	Simetrično rješ. $u(x)$	Asim. rješ. $u(x)$
(1)	Be^{lx}	Be^{lx}
(2)	$A\cos kx$	$A\sin kx$
(3)	Be^{-lx}	$-Be^{-lx}$

2° neprekinutost valne fje. $u(x)$ na $\frac{a}{2}$ & $-\frac{a}{2}$ i npr. $u'(x)$

Sim. rješ.: $x=\frac{a}{2}$ $\quad A\cos k\frac{a}{2} = Be^{-\frac{la}{2}} \qquad -Ak\sin\frac{ka}{2} = -Ble^{-\frac{la}{2}} \Rightarrow$

nepotrebno $x=-\frac{a}{2}$ $\quad A\cos k\frac{a}{2} = Be^{-\frac{la}{2}} \qquad -Ak\sin\frac{ka}{2} = Ble^{-\frac{la}{2}}$

$\Rightarrow \operatorname{tg}\frac{ka}{2} = \frac{l}{k}$

$$\boxed{\operatorname{tg}\frac{ka}{2} = \frac{l}{k}} \quad i)$$

$\operatorname{tg}\frac{ka}{2} = \frac{l}{k}$ i)

Asim. rješ: $x = \frac{a}{2}$ $\quad u(x)$ $\quad A\sin\frac{ka}{2} = -Be^{-\frac{la}{2}}$

$u'(x)$ $\quad Ak\cos\frac{ka}{2} = Bl\,e^{-\frac{la}{2}}$

$$\Bigg\} \Rightarrow \underline{\operatorname{tg}\frac{ka}{2} = -\frac{k}{l}} \qquad \text{ii)}$$

i) & ii) transcendentne jbe. Kod danu uvjet na energiju E

$l^2 = \frac{2m}{\hbar^2}|E|$ $\quad k^2 = \frac{2m}{\hbar^2}(-U_0 - |E|)$

$$k^2 + l^2 = \frac{2m}{\hbar^2}(\underset{\vee\,0}{-U_0}) = \frac{2m}{\hbar^2}|U_0| = \frac{(2\alpha)^2}{a^2} \qquad \text{tj. } \alpha^2 = \frac{m|U_0|}{2\hbar^2}a^2$$

$\alpha^2 \sim a^2 \cdot |U_0|$ – mjeri „volumen" pot. jame

$$l = \sqrt{\frac{(2\alpha)^2}{a^2} - k^2} = \frac{2}{a}\sqrt{\alpha^2 - \left(\frac{ka}{2}\right)^2} \Rightarrow \frac{l}{k} = \frac{\sqrt{\alpha^2 - \left(\frac{ka}{2}\right)^2}}{\frac{ka}{2}}$$

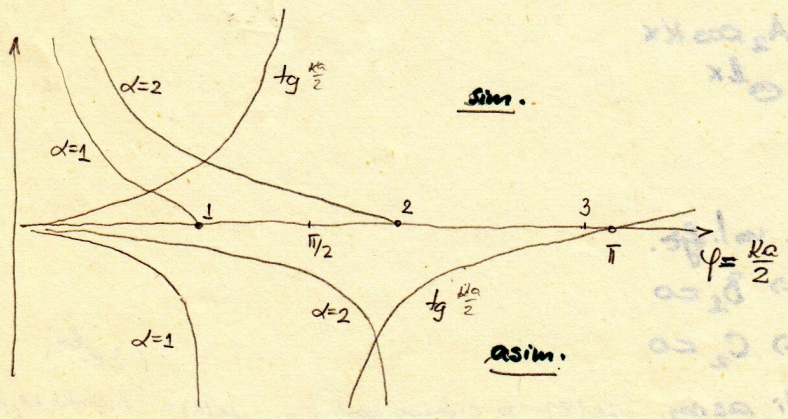
$\frac{ka}{2} = \varphi$

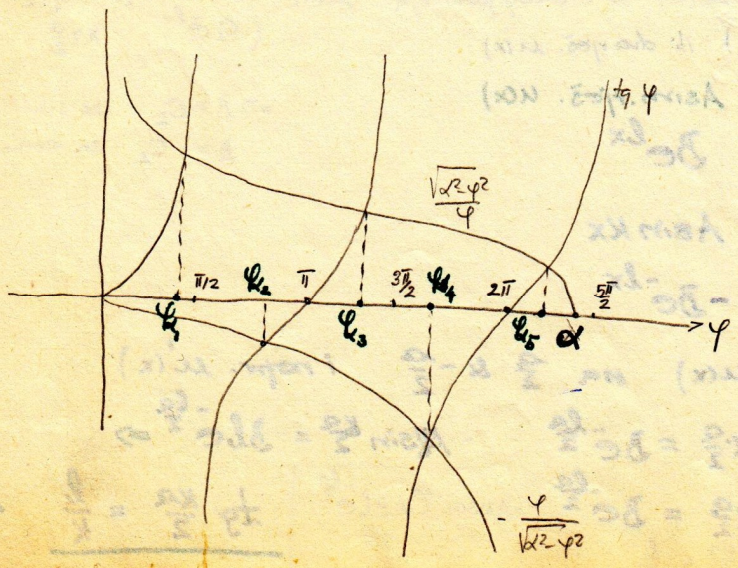
Sim: $\operatorname{tg}\varphi = \frac{\sqrt{\alpha^2 - \varphi^2}}{\varphi}$ $\qquad$ Asim: $\operatorname{tg}\varphi = -\frac{\varphi}{\sqrt{\alpha^2 - \varphi^2}}$

$k^2 = \frac{2m}{\hbar^2}(|U_0| - |E|) > 0 \Rightarrow \frac{ka}{2} \geq 0$

$|U_0| > |E|$

$$\left.\begin{array}{l} \frac{k^2a^2}{2^2} = \alpha^2 - \left(\frac{al}{2}\right)^2 \Rightarrow \frac{ka}{2} = \sqrt{\alpha^2 - \left(\frac{al}{2}\right)^2} \\ l^2 = \frac{2m}{\hbar^2}|E| \geq 0 \quad \begin{smallmatrix} E\neq 0 \\ E=0 \end{smallmatrix} \end{array}\right\} \Rightarrow \frac{ka}{2} \leq \alpha \Bigg\} \Rightarrow \underline{0 \leq \varphi \leq \alpha}$$





$n = 1, 2, \ldots$ ograničeno

$$(\varphi_\alpha^2)_n = \frac{k^2 a^2}{4} = \frac{a^2}{4} \cdot \frac{2m}{\hbar^2}(|U_0| - |E|)$$

$$\Rightarrow \quad |U_0| - |E| = \frac{2\hbar^2}{ma^2} \cdot (\varphi_\alpha^2)_n$$

n - ograničen sa α

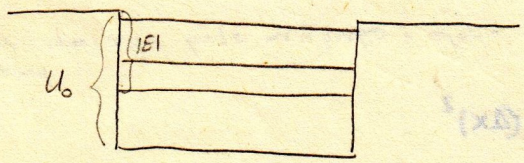
tj. $(\varphi_\alpha)_{n_{max}} < \alpha \qquad \alpha^2 = \frac{m|U_0|}{2\hbar^2} a^2$

→ što je veći „volumen" pot. jame to je veći broj rješ. φ_α

tj. veći broj diskretnih vrijednosti energije E

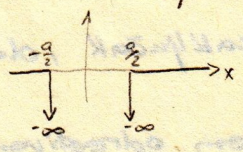
Sapok Th. $\exists$ najviši term za $(\varphi_\alpha)_{max}$ iznad kojeg se proteže kontinuum pozitivnih energija. (Čestice pozitivne energije prolete preko pot. jame).

sa grafova ⇒ - ako je jama suviše plitka, nećete u njoj za asim. valnu fju. biti niti jedan term energije, što znači, da čestica nije više vezana (tj. slobodno se giba, jer na nju pot. energija ne vrši nikakav utjecaj).



Za $U_0 \to \infty \Rightarrow \alpha \to \infty$

- moramo dobiti isto kao da direktno rješavamo Schröd. jbu. za slučaj



izradi !!!

sim. $\quad tg\,\varphi = \frac{\sqrt{\alpha^2 - \varphi^2}}{\varphi} \to \infty \qquad \varphi = (2n+1)\frac{\pi}{2}$

asim. $\quad tg\,\varphi = -\frac{\varphi}{\sqrt{\alpha^2 - \varphi^2}} \to 0 \qquad \varphi = (2n)\cdot\frac{\pi}{2}$

sim. $\quad |U_0| - |E| = \frac{\hbar^2 \pi^2}{2ma^2}(2n+1)^2$

asim. $\quad |U_0| - |E| = \frac{\hbar^2 \pi^2}{2ma^2}(2n)^2$

U fizici - titranja → harmonijska (model H.O.)

1) el. magn. valovi
2) 2-A mol.
3) ioni u kristalu
4) Jezgre
5) Plazma

Harmonički oscilator (1-D)

klasični hamilt. $H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2$

informacije iz relac. neodređenosti

$$\Delta p \cdot \Delta x \approx h$$

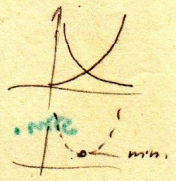
→ za najniže energetsko stanje - koje i egzistira zbog $\Delta p \cdot \Delta x \approx h$ u atomu, a ne padne ē na jezgru

radi veličine

$$E_0 \approx \frac{(\Delta p)^2}{2m} + \frac{m\omega^2}{2}(\Delta x)^2$$

$$\approx \frac{h^2}{2m(\Delta x)^2} + \frac{m\omega^2}{2}(\Delta x)^2$$

⇒ zaključak, da E_0 ne može biti proizvoljno mala! jer



Problem određivanja minimuma E_0

$$\frac{dE_0}{d(\Delta x)} = 0 = -\frac{h^2}{m(\Delta x)^3} + m\omega^2(\Delta x)$$

$$\Rightarrow (\Delta x)^4 = \left(\frac{h}{m\omega}\right)^2$$

$$E_0 \approx \frac{h^2}{2m \cdot \frac{h}{m\omega}} + \frac{m\omega^2}{2} \cdot \frac{h}{m\omega} = \hbar\omega$$ - grubo rješenje

naime: $E_n = \frac{\hbar\omega}{2}(2n+1)$ na vježbama str. 5. sa računanjem matrice $H = [(H_{nn}\delta_{nm})]_{nm}$

$$\Rightarrow E_0 = \frac{\hbar\omega}{2}$$ direktna posljedica

→ zbog relacija neodređenosti čestica barem malo titra oko ravnotežnog položaja

→ egzaktni račun - rješ. Schröd. jbe.

$$\frac{d^2u(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E - U(x)\right)u(x) = 0$$

$$U(x) = \frac{m\omega^2}{2}x^2$$

- prikladna varijabla : def: $a = \sqrt{\frac{\hbar}{m\omega}}$ $\qquad \frac{2m}{\hbar^2}\cdot\frac{m\omega^2}{2} = \left(\frac{m\omega}{\hbar}\right)^2 = \frac{1}{a^4}$ ←

$\frac{\hbar\omega}{m\omega^2}$ $\qquad \sqrt{\frac{m}{g}\cdot s} = \sqrt{\frac{m}{g}\cdot s^2} = \sqrt{\frac{g\omega^2 s^2}{g}\cdot s^2} = m$

energiju mjerimo sa :

$$E = \frac{\hbar\omega}{2}\cdot K$$

bezdimenzionalna veličina - kont. ili diskretin. ?

$$\frac{2m}{\hbar^2}E = \frac{2m}{\hbar^2}\cdot\frac{\hbar\omega}{2}\cdot K = \frac{m\omega}{\hbar}K = \frac{K}{a^2}$$

$$\Rightarrow \quad \frac{d^2u}{dx^2} + \left(\frac{K}{a^2} - \frac{x^2}{a^4}\right)u = 0$$

$[a]$ = dužina

$\frac{du(x)}{dx} = \frac{du(as)}{dx} = \frac{1}{a}\frac{du(as)}{ds}$

def : bez dimenz. veliči. $\quad s = \frac{x}{a} \quad \Rightarrow \quad \frac{du}{dx} = \frac{du}{a\,ds}$ $\qquad u(x) = u(as) = u_1(s)$

$$u' = \frac{du}{ds} \qquad \frac{d^2u}{dx^2} = \frac{1}{a^2}\frac{d^2u}{ds^2}$$

$\frac{1}{a^2}u'' + \left(\frac{K}{a^2} - \frac{s^2}{a^2}\right)u = 0$

$$\Rightarrow \quad u''_{(as)} + (K - s^2)u_{(as)} = 0$$

rješavamo u cijelom području

$-\infty \le s \le +\infty$

$U(-x) = U(x)$

& $R = \pm\infty \quad U(R) = \infty \Rightarrow u(R) = 0 \Rightarrow u_2(x) = C\,u_1(x)$

str. 24 $\xRightarrow{(*)}$ $u(x) = \pm u(-x)$ $\quad (*)'$!!nedovoljno

1° Konačnost valne fje.

za $x \to \pm\infty \quad U \to \infty \Rightarrow u \to 0$ tj. $u(\pm\infty) = 0$

→ asimptotsko ponašanje:

za $s \to \infty$ tj. tada $K \lll s$

$$\Rightarrow \quad u''_{(as)} - s^2 u_{(as)} = 0 \qquad \Rightarrow \text{ približno rješenje}$$

ili $u_1''(s) - s^2 u_1(s) = 0$

$u''(s) - s^2 u_I(s) = 0$

→ probn. rješenje $\underline{u = e^{-\frac{s^2}{2}}}$ (*) $u' = -s e^{-\frac{s^2}{2}}$ $u'' = e^{-\frac{s^2}{2}}(-1+s^2)$

$$u'' - s^2 u = e^{-\frac{s^2}{2}}(-1+s^2) - s^2 e^{-\frac{s^2}{2}} = -e^{-\frac{s^2}{2}} \to 0 \text{ jer } s \to \infty$$

⇒ (*) aproksimativno rješenje za $\forall K$

→ isto tako može $u = e^{\frac{s^2}{2}}$ ali to je samo matem. rješ., a ne i fizikalno jer $u(\pm\infty) = 0$

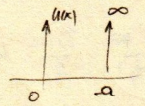
→ (*) je egzaktno rješenje za $K=1$

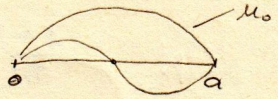
$$u_1''(s) + (1-s^2)u_1(s) = e^{-\frac{s^2}{2}}(-1+s^2) + (1-s^2)e^{-\frac{s^2}{2}} = 0$$

$$\Rightarrow \underline{u_0(s) = e^{-\frac{s^2}{2}}} \qquad \underline{E_0 = \frac{\hbar\omega}{2}}$$

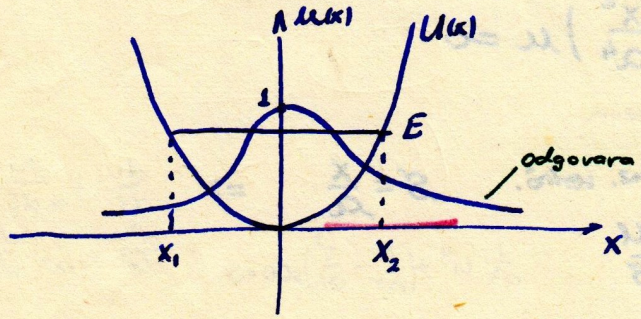
$u_1(s) - u(x) = e^{-\frac{x^2}{2a^2}}$

– u problemu





možimo



odgovara rješenju bez čvorišta i isto prva valna fja. sim. s obzirom na ishodište kao i $U(x)$

→ { Klas.: čestica se nalazi samo između x_1 & x_2 gdje $E > U$
{ Kvant.: i izvan x_1 & x_2 ali šansa exp. pada – (približna formula na (23))

ili preko gustoće vjerojatnosti $\rho = |\psi|^2 = u^2(x) \to 0$ za $x \to \pm\infty$

original!!!

1° $E = U(x) \Rightarrow \frac{\hbar\omega}{2} = \frac{m\omega^2}{2} x_{1,2}^2 \Rightarrow x_1^2 = x_2^2 = \frac{\hbar}{m\omega} = a^2 \Rightarrow |x_1| = |x_2| = a$

2° $u_0(x) = e^{-\frac{x^2}{2a^2}}$ (*) $u_0(x_{1/2}) = \frac{1}{e}$ (*) $\Rightarrow -\frac{x^2}{2a^2} = -1 \Rightarrow x^2 = 2a^2 \Rightarrow x_{1/2} = \sqrt{2}\,a$

širina maximuma

} istog reda veličine ⇒

⇒ izrazita gustoća vjerojatnosti je baš između x_1 & x_2

$u_1''(s) + (K - s^2)\, u_1(s) = 0$

→ pokusno rješenje:

$$u_1(s) = e^{-\frac{s^2}{2}} H_n(s)$$

$u_1'(s) = -s\, e^{-\frac{s^2}{2}} H_n(s) + e^{-\frac{s^2}{2}} H_n'(s)$

$u_1''(s) = -e^{-\frac{s^2}{2}} H_n(s) + s^2 e^{-\frac{s^2}{2}} H_n(s) - s e^{-\frac{s^2}{2}} H_n'(s) - s e^{-\frac{s^2}{2}} H_n'(s) + e^{-\frac{s^2}{2}} H_n''(s)$

$$u(x) = u_1''(s) = H_n''(s) e^{-\frac{s^2}{2}} - 2s e^{-\frac{s^2}{2}} H_n'(s) + (s^2 - 1) e^{-\frac{s^2}{2}} H_n(s)$$

!!. ...pro

$$+ (K - s^2) e^{-\frac{s^2}{2}} H_n(s) = 0 \quad / : e^{-\frac{s^2}{2}} \neq 0 \text{ za } s \neq \pm\infty$$

kad je značajan $H_n(s)$

$$\Rightarrow H_n'' - 2s H_n' + (K-1) H_n = 0$$

→ pretp. rješ. kao razvoj u red

$$H_n(s) = \sum_{m=0}^{n} C_m s^m$$

napomena !!!

→ naime ukupno rješ. $u_1(s)$ nisu svi pretp. u tom obliku jer ne bi konvergiralo za $s \to \pm\infty$ dok $\lim_{x\to\pm\infty} x^m e^{-x^2} = 0 \ \forall m$

→ taj faktor će dati ispravan broj čvorišta (kao i ba. n-tog stupnja)

→ faktor $e^{-\frac{s^2}{2}}$ omogućuje da se rješ. ispravno ponaša na velikim udaljenostima

→ ne mogu doći potencije:

$\frac{1}{s}$ tj. $m < 0$ jer rješ. ne bi bilo konačno za $s \to 0$

čak $s^{1/2}$ tj. $0 < m < 1$ jer ne bi postojala mogućnost za $\exists$ sim. i asim. rješ. tj. takvo rješ. ne bi moglo mijenjati predznak (asim. rješ) za $s \to -s$ ili uopće ne bi bilo realno

→ $c_0 = c_2 = c_4 = \dots = 0$ asim. rješ

$c_1 = c_3 = c_5 = \dots = 0$ sim. rješ. } *)

rub $R = \pm\infty$

$u(\pm\infty) = 0$

→ tm. o regularnosti (24) ili (*) u (24) (*) ⇒ samo jedno rješ. zadovoljava uvjet regularnosti tj. ili je sim. ili asim. rješ.

$m \to m+1$

$$H_n' = \sum_{m=1}^{n} m C_m s^{m-1} = \sum_{m=0}^{n-1} (m+1) C_{m+1} s^m$$

$$H_n'' = \sum_{m=2}^{n} m(m-1) C_m s^{m-2} = \sum_{m=0}^{n-2} (m+2)(m+1) C_{m+2} s^m$$

$m \to m'+2$

$m = 2 \to m' = 0$

$m = n \to m' = n-2$

$$\sum_{m=0}^{n-2} C_{m+2}(m+2)(m+1) s^m - 2s \sum_{m=1}^{n} m C_m s^{m-1} + (K-1) \sum_{m=0}^{n} C_m s^m = 0$$

$m \to m = 0$

$2C_2 + (K-1) C_0 = 0$

$$\sum_{m=0}^{n-2} s^m \underbrace{\left[C_{m+2}(m+2)(m+1) - C_m \cdot 2m + C_m (K-1) \right]}_{=0} + C_{n-1} \cdot \underbrace{(-2(n-1) + K - 1)}_{(K-(2n-1))} s^{n-1} + C_n \underbrace{(-2n + K - 1)}_{(K-(2n+1))} s^n = 0$$

$\forall s \Rightarrow$

!!! ovdje

*) ⇒ asim. rješ. odred. sa C_1

sim. rješ. odred. sa $C_0 = -2$

$$\Rightarrow \text{rekurzivna relacija} \quad C_{m+2} = \frac{2m + 1 - K}{(m+2)(m+1)} C_m \quad i)$$

iii) $C_{n-1}[K - (2n-1)] = 0$

& iii)' $C_n [K - (2n+1)] = 0$

zbog fc. izvodnice

ovg.

poč. vrijednosti C_0 & C_1 odredjuju dva lin. nezav. rješenja

Treba pokazati da je samo jedno rješ. regularno.

→ dokaz da je samo jedno rješenje za $H_n(s)$ regularno i to kad je $H_n(s)$ polinom n-tog stupnja, a ne ∞ polinom tj. fja.

pogledajmo razvoj

$$\frac{s^{2m}}{m!} \qquad \frac{s^{2(m+1)}}{(m+1)!} = \frac{s^{2m+2}}{(m+1)!}$$

$$e^{s^2} = 1 + \frac{s^2}{1!} + \frac{s^4}{2!} + \dots + \frac{s^m}{(\frac{m}{2})!} + \frac{s^{m+2}}{(\frac{m}{2}+1)!} + \dots = \sum_m b_m s^m$$

$m = 0, 2, 4, 6, \dots$

$$\frac{b_{m+2}}{b_m} = \frac{\frac{1}{(\frac{m}{2}+1)!}}{\frac{1}{(\frac{m}{2})!}} = \frac{1}{\frac{m}{2}+1} \xrightarrow[\text{za } m \gg 1]{\text{asimptot. ponašanje}} \frac{2}{m}$$

može za $n \gg 1$

Vratimo se:

$$\frac{C_{m+2}}{C_m} = \frac{2m+1-K}{(m+2)(m+1)} \xrightarrow[\text{tj. } m \gg K]{m \gg 1} \frac{2}{m}$$

$\frac{2m}{m^2}$

može kad: $n \gg 1$

⇒ orig. !!! Ako m može biti po volji veliko tj. i sam n tada bi trebalo regularnosti zadovoljavati takoder i e^{s^2}, jer se slično ponašaju njegovi koef. za $m \gg 1$

orig.: ⇒ asimptotsko ponašanje za $u(s)$ tj. $s \to \pm\infty$

$$u(s) = e^{-\frac{s^2}{2}} \cdot e^{s^2} = e^{\frac{s^2}{2}} \to \infty$$

⇒ odgovara rješenje za $H_n(s)$ kod kojeg m tj. n ne može po volji rasti

orignalno!!!

tip rješenja

I n-paran

sim: $C_n \neq 0 \overset{iii)'}{\Rightarrow} K = 2n+1$ $\quad n = 0, 2, 4, \dots \overset{i)}{\Rightarrow} C_{n+2} = 0$ — što mora biti ispunjeno

$C_{n-1} = 0 \overset{i)}{\Rightarrow} C_{n+1} = 0$

asim: $C_{n-1} \neq 0 \overset{iii)}{\Rightarrow} K = 2n-1$ $\quad n = 2, 4, 6, \dots \overset{i)}{\Rightarrow} C_{n+1} = 0$

(za $n=0$ nema asim. rješ.)

$C_n = 0 \overset{i)}{\Rightarrow} C_{n+2} = 0$

ustvari polinom $(n-1)$ stupnja $\Rightarrow K = 2n-1 = 2(n-1)+1$

II n-neparan

sim: $C_{n-1} \neq 0 \overset{iii)}{\Rightarrow} K = 2n-1$ $\quad n = 1, 3, 5, 7, \dots \overset{i)}{\Rightarrow} C_{n+1} = 0$

$C_n = 0 \overset{i)}{\Rightarrow} C_{n+2} = 0$

asim: $C_n \neq 0 \overset{iii)'}{\Rightarrow} K = 2n+1$ $\quad n = 1, 3, 5, 7, \dots \overset{i)}{\Rightarrow} C_{n+2} = 0$

$C_{n-1} = 0 \overset{i)}{\Rightarrow} C_{n+1} = 0$

$\Rightarrow K = 2n+1$

$n = 0, 1, 2, 3, \dots$

$$\Rightarrow E_n = \frac{\hbar\omega}{2}(2n+1) \qquad n = 0, 1, 2, 3, 4, \dots$$

$H_n'' - 2s H_n' + (K-1) H_n = 0$

bilo!!!

$\left.\begin{array}{l} n\text{-paran \& sim.} \\ n\text{-neparan \& asim} \end{array}\right\} \Rightarrow K = 2n+1 \Rightarrow H_n'' - 2s H_n' + 2n H_n = 0$

$\left.\begin{array}{l} n\text{-paran \& asim.} \\ n\text{-neparan \& sim.} \end{array}\right\} \Rightarrow K = 2n-1 \Rightarrow H_n'' - 2s H_n' + 2(n-1) H_n = 0$

$H_n(s) = (-1)^n H_n(-s)$ ←

Hermite-ovi polinomi

Šepek II 737-738: 8, 9, 10

Arsenin

napomena: za $H_n(s)$

n-paran ima samo parne potencije

n-neparan ima samo neparne potencije

Hermite-ovi polinomi

n-paran & sim.
n-nepar. & asim.

bitno!!!

$$C_{m+2} = \frac{2m+1-K}{(m+2)(m+1)} C_m \qquad K = 2n+1$$

$$C_{m+2} = -2\,\frac{n-m}{(m+2)(m+1)}\, C_m \qquad m = 0,1,2,\dots n$$

$$H_n(s) = \sum_{m=0}^{n} C_m s^m \qquad C_0 = -2 \quad 12 \qquad C_1 = -2 \quad -12$$

$\Rightarrow$ $C_0 = 1$ $\quad H_0 = 1$ zapravo $H_0 = -2$ ali C_0 je ionako proizv. odabran

$C_1 = 2$ $\quad H_1 = 2s$ – ovdje $C_1 = 2$

$C_0 = -2$ $\quad H_2 = 4s^2 - 2$

$C_1 = -12$ $\quad H_3 = 8s^3 - 12s$

$C_0 = 12$ $\quad H_4 = 16s^4 - 48s^2 + 12$

$\vdots$

$C_2 = -2\,\frac{2-0}{2}\cdot C_0 = -2\cdot(-2) = 4$

$C_3 = -2\,\frac{3-1}{3\cdot 2}\, C_1 = -\frac{2}{3}(-12) = +8$

$C_0 = 12 \quad C_2 = -2\,\frac{4-0}{2}\cdot 12 = -48 \quad C_4 = -2\cdot\frac{4-2}{4\cdot 3}\cdot(-48) = -2\cdot 2\cdot(-4) = 16$

Fja. izvodnica:

$$\phi(s,t) = e^{2st-t^2} = \sum_{n=0}^{\infty} H_n(s)\cdot\frac{t^n}{n!} \qquad \Big/ \frac{\partial}{\partial s}$$

Supek II 737.

$$2t\, e^{2st-t^2} = \sum_{n=0}^{\infty} H_n'(s)\,\frac{t^n}{n!}$$

$$\Rightarrow \phi(s,t) = e^{2st-t^2} = \sum_{n=0}^{\infty} \frac{H_n'(s)}{2n}\,\frac{t^{n-1}}{(n-1)!} \qquad \Rightarrow \quad H_n'(s) = 2n\, H_{n-1}(s)$$

$$H_{n-1}(s) = \frac{1}{2n} H_n'(s)$$

$$(2s-2t)\underbrace{e^{2st-t^2}}_{\phi(s,t)} = \sum_{n=1}^{\infty} H_n(s)\cdot\frac{t^{n-1}}{(n-1)!}$$

$$\Rightarrow \sum_{n=1}^{\infty}\left[H_n(s)\cdot\frac{t^{n-1}}{(n-1)!} - 2s H_n(s)\frac{t^n}{n!} + 2H_n(s)\cdot\frac{(n-1)\, t^{n+1}}{n!\,(n-1)}\right] = 0$$

$$\sum_{n=1}^{\infty} H_n(s)\frac{t^{n-1}}{(n-1)!} + \sum_{n=1}^{\infty} -2s H_{n-1}(s)\frac{t^{n-1}}{(n-1)!} + \sum_{n=2}^{\infty} 2(n-1) H_{n-2}\frac{t^{n-1}}{(n-1)!} = 0$$

$$\underbrace{H_1(s) - 2s\, H_0(s)}_{=0\ (2s - 2s\cdot 1 = 0)} + \sum_{n=2}^{\infty}\left[H_n(s) - 2s H_{n-1}(s) + 2(n-1) H_{n-2}\right]\frac{t^{n-1}}{(n-1)!} = 0$$

$$\Rightarrow \quad H_n(s) - 2s\, H_{n-1}(s) + 2(n-1) H_{n-2}(s) = 0 \qquad H_{n-2}(s) = \frac{1}{2(n-1)} H_{n-1}'(s) = \frac{1}{4n(n-1)} H_n''(s)$$

$$H_n(s) - 2s\cdot\frac{1}{2n} H_n'(s) + 2(n-1)\cdot\frac{1}{4n(n-1)} H_n''(s) = 0 \quad /2n$$

$$\Rightarrow \quad H_n'' - 2s H_n' + 2n H_n = 0$$ jba. za Hermiet-ove polinome

općenito:

$$H_n(s) = (-1)^n H_n(-s)$$

$$\phi(s,t) = e^{2st-t^2} = \sum_m H_m \frac{t^m}{m!}$$

$$H_n(s) = \left[\frac{\partial^n}{\partial t^n} \sum_{m=0}^{\infty} H_m(s) \frac{t^m}{m!}\right]_{t=0} = \left[\frac{\partial^n}{\partial t^n} e^{2st-t^2}\right]_{t=0}$$

$$\left[\frac{\partial}{\partial t} e^{2st-t^2}\right]_{t=0} = e^{s^2}\left[\frac{\partial}{\partial t} e^{-(s-t)^2}\right]_{t=0} = -e^{s^2}\left[\frac{\partial}{\partial s} e^{-(s-t)^2}\right]_{t=0} = -e^{s^2}\frac{\partial}{\partial s} e^{-s^2}$$

$$\frac{\partial^n}{\partial t^n} e^{2st-t^2} = (-1)^n e^{s^2}\left[\frac{\partial^n}{\partial s^n} e^{-(s-t)^2}\right]$$

$$\Rightarrow \quad H_n(s) = (-1)^n e^{s^2} \frac{d^n}{ds^n} e^{-s^2}$$

→ rješenje H. O.

$$s = \frac{x}{a} \qquad a = \sqrt{\frac{\hbar}{m\omega}}$$

$$u_n(x) = A_n e^{-\frac{s^2}{2}} H_n(s)$$

$$\int |\psi|^2 d\tau = 1 \quad \Rightarrow \quad \int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx = \delta_{mn} \qquad *)$$

$a\, ds$

dokaz: ortogonalnosti & odred. A_n

→ def. dvije fje izvodnice

$$\phi_i(s,t_i) = e^{2st_i - t_i^2} = \sum_{n=0}^{\infty} H_n(s) \frac{t_i^n}{n!} \qquad i = 1,2$$

n, m sumacija

$$2t_1t_2 \qquad -2t_1t_2$$

$$-s^2 + 2st_1 - t_1^2 + 2st_2 - t_2^2 = -[s^2 - 2s(t_1+t_2) + (t_1+t_2)^2]$$

$$\int_{-\infty}^{\infty} \phi_1 \cdot \phi_2\, e^{-s^2} ds = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{t_1^n}{n!}\frac{t_2^m}{m!} \underbrace{\int_{-\infty}^{\infty} H_n(s)\cdot H_m(s)\, e^{-s^2} ds}_{= e^{2t_1t_2}\int_{-\infty}^{\infty} e^{-(s-t_1-t_2)^2} d(s-t_1-t_2)}$$

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

$$= e^{2t_1t_2}.$$

$$= \sum_{n=0}^{\infty} \frac{\sqrt{\pi}}{n!} (2t_1t_2)^n.$$

$$\Rightarrow \quad \int_{-\infty}^{\infty} H_n(s) H_m(s)\, e^{-s^2} ds = n!\, 2^n \sqrt{\pi}\, \delta_{nm}$$

$$*) \Rightarrow \quad \cancel{|A_n|^2}\ A_n^* \cdot A_n \int_{-\infty}^{\infty} e^{-\frac{s^2}{2}} H_n(s)\, e^{-\frac{s^2}{2}} H_m(s)\, a\, ds = n!\, 2^n \sqrt{\pi}\, \delta_{nm}$$

$$\Rightarrow \quad A_n = \frac{1}{\sqrt{2^n n!\, a \sqrt{\pi}}}$$